



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 02:47 AM EDT

PDB ID : 6U7L  
Title : 2.75 Angstrom Crystal Structure of Galactarate Dehydratase from Escherichia coli.  
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Deposited on : 2019-09-03  
Resolution : 2.75 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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	:	2.37.1
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)	:	2.37.1

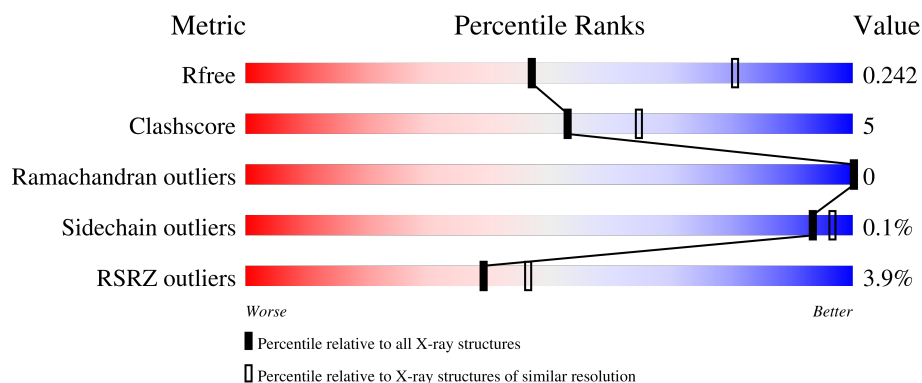
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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  $\geq 3$ , 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	526	<div> <div>3%</div> <div>78%</div> <div>9%</div> <div>13%</div> </div>
1	B	526	<div> <div>3%</div> <div>73%</div> <div>12%</div> <div>14%</div> </div>
2	C	526	<div> <div>2%</div> <div>79%</div> <div>7%</div> <div>14%</div> </div>
2	D	526	<div> <div>6%</div> <div>76%</div> <div>10%</div> <div>14%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14035 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 Galactarate dehydratase (L-threo-forming).

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	P	S	Se	0	1	0
			3506	2229	600	661	1	6	9			
1	B	451	Total	C	N	O	P	S	Se	0	0	0
			3453	2197	590	651	1	5	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P39829
A	-1	ASN	-	expression tag	UNP P39829
A	0	ALA	-	expression tag	UNP P39829
B	-2	SER	-	expression tag	UNP P39829
B	-1	ASN	-	expression tag	UNP P39829
B	0	ALA	-	expression tag	UNP P39829

- Molecule 2 is a protein called Galactarate dehydratase (L-threo-forming).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	453	Total	C	N	O	S	Se	0	0	0
			3455	2200	592	649	5	9			
2	D	452	Total	C	N	O	S	Se	0	1	0
			3455	2201	592	648	5	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP P39829
C	-1	ASN	-	expression tag	UNP P39829
C	0	ALA	-	expression tag	UNP P39829
D	-2	SER	-	expression tag	UNP P39829
D	-1	ASN	-	expression tag	UNP P39829
D	0	ALA	-	expression tag	UNP P39829

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Cl 4 4	0	0
4	D	3	Total Cl 3 3	0	0

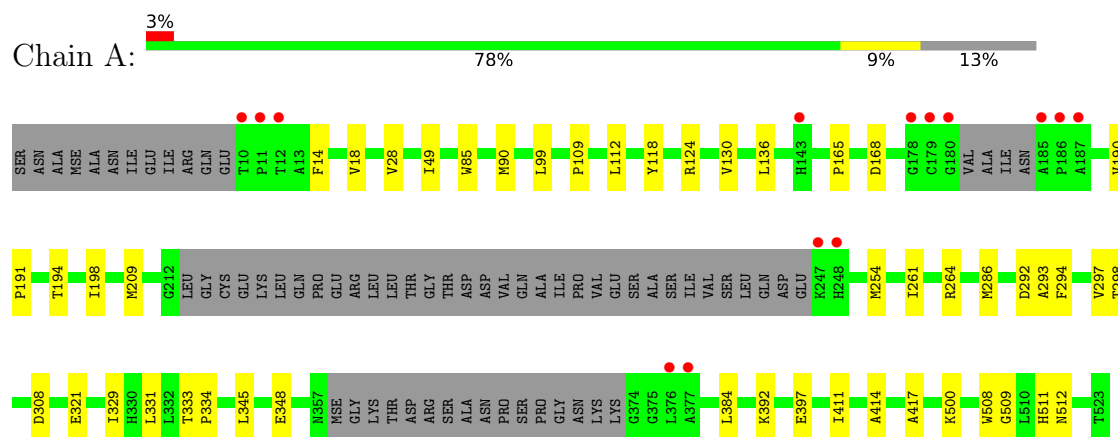
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	41	Total O 41 41	0	0
5	B	25	Total O 25 25	0	0
5	C	52	Total O 52 52	0	0
5	D	32	Total O 32 32	0	0

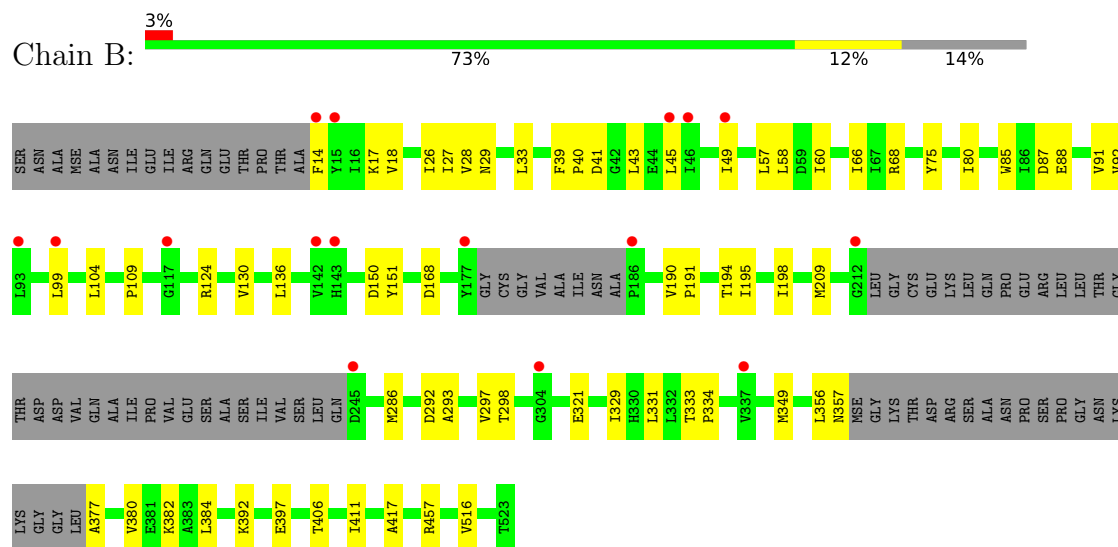
### 3 Residue-property plots

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.

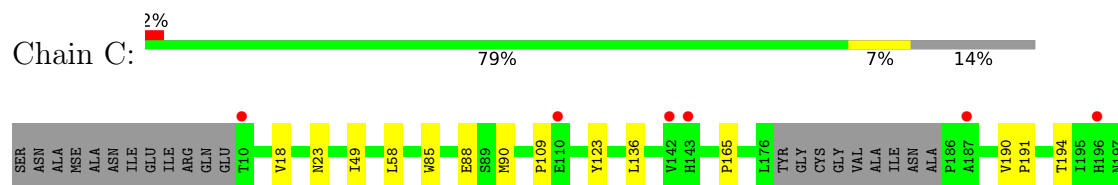
- Molecule 1: Galactarate dehydratase (L-threo-forming)

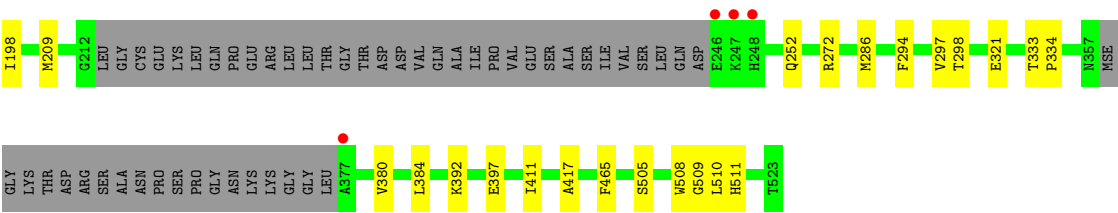


- Molecule 1: Galactarate dehydratase (L-threo-forming)

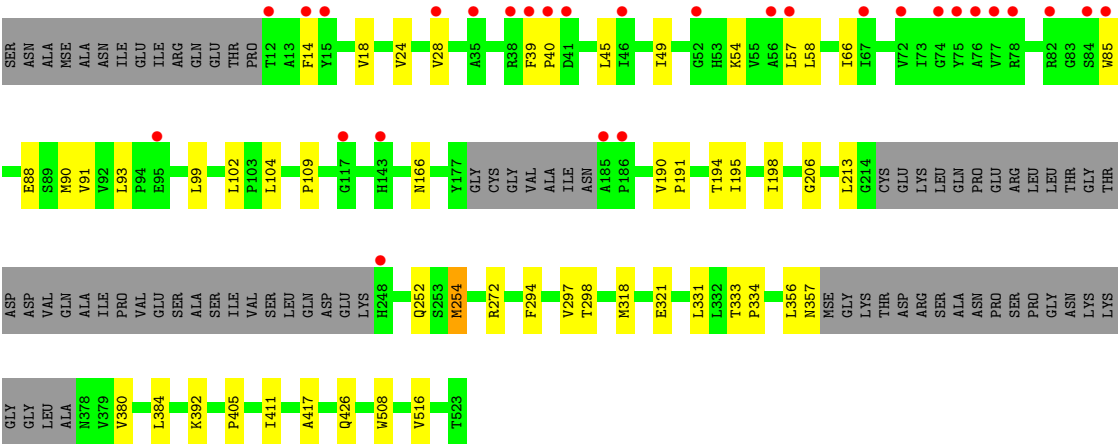
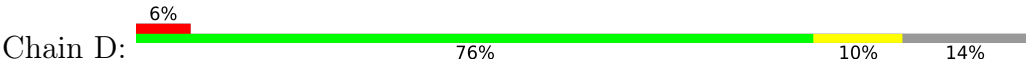


- Molecule 2: Galactarate dehydratase (L-threo-forming)





● Molecule 2: Galactarate dehydratase (L-threo-forming)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.46Å 167.57Å 117.06Å 90.00° 103.97° 90.00°	Depositor
Resolution (Å)	29.23 – 2.75 29.23 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.23-2.75) 98.9 (29.23-2.75)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.206 , 0.241 0.208 , 0.242	Depositor DCC
$R_{free}$ test set	2734 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.2	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 31.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CL, PHD, CA

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	0.65	0/3557	0.73	3/4826 (0.1%)
1	B	0.65	0/3503	0.73	1/4751 (0.0%)
2	C	0.65	0/3518	0.73	2/4775 (0.0%)
2	D	0.66	0/3518	0.73	2/4776 (0.0%)
All	All	0.65	0/14096	0.73	8/19128 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	286	MSE	CG-SE-CE	5.95	112.00	98.90
1	A	254	MSE	CG-SE-CE	5.87	111.81	98.90
2	C	90	MSE	CG-SE-CE	5.68	111.39	98.90
1	A	286	MSE	CG-SE-CE	5.65	111.33	98.90
2	D	90	MSE	CG-SE-CE	5.49	110.97	98.90
1	A	90	MSE	CG-SE-CE	5.47	110.93	98.90
1	B	286	MSE	CG-SE-CE	5.45	110.89	98.90
2	D	254	MSE	CG-SE-CE	5.27	110.49	98.90

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	3506	0	3508	35	0
1	B	3453	0	3455	52	0
2	C	3455	0	3469	27	0
2	D	3455	0	3463	44	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	4	0	0	0	0
4	D	3	0	0	0	0
5	A	41	0	0	0	0
5	B	25	0	0	0	0
5	C	52	0	0	0	0
5	D	32	0	0	2	0
All	All	14035	0	13895	150	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 (150) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ILE:CD1	1:B:49:ILE:HB	2.16	0.74
2:D:66:ILE:CD1	2:D:91:VAL:HG12	2.19	0.72
2:D:93:LEU:HD12	2:D:93:LEU:O	1.92	0.69
1:B:329:ILE:HG21	1:B:349:MSE:SE	2.43	0.69
1:A:348:GLU:HG2	1:A:414:ALA:HB2	1.79	0.64
2:D:318:MSE:HE1	2:D:426:GLN:HA	1.80	0.63
1:B:39:PHE:HB3	1:B:40:PRO:HD2	1.81	0.63
2:D:213:LEU:C	2:D:213:LEU:HD23	2.21	0.61
2:C:252:GLN:NE2	2:D:508:TRP:CD2	2.68	0.61
1:A:112:LEU:HD12	1:A:112:LEU:N	2.15	0.60
1:A:348:GLU:HG2	1:A:414:ALA:CB	2.31	0.60
1:B:66:ILE:HD12	1:B:91:VAL:HG23	1.81	0.60
1:B:190:VAL:HB	1:B:191:PRO:HD3	1.84	0.59
2:D:104:LEU:HD12	2:D:104:LEU:N	2.17	0.59
2:D:39:PHE:HB3	2:D:40:PRO:HD2	1.85	0.59
2:C:190:VAL:HB	2:C:191:PRO:HD3	1.85	0.59
2:C:252:GLN:NE2	2:D:508:TRP:CE3	2.70	0.59
1:B:27:ILE:HD11	1:B:49:ILE:HB	1.83	0.59
1:B:104:LEU:N	1:B:104:LEU:HD12	2.16	0.59
1:A:190:VAL:HB	1:A:191:PRO:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:99:LEU:HD12	2:D:99:LEU:N	2.18	0.58
2:D:88:GLU:OE1	2:D:88:GLU:N	2.35	0.58
2:D:190:VAL:HB	2:D:191:PRO:HD3	1.85	0.57
1:B:60:ILE:CG1	1:B:80:ILE:HB	2.35	0.57
2:D:24:VAL:CG1	2:D:54:LYS:HB2	2.35	0.57
1:A:99:LEU:HD12	1:A:99:LEU:N	2.20	0.56
2:C:88:GLU:N	2:C:88:GLU:OE1	2.36	0.56
2:C:397:GLU:HB3	2:C:411:ILE:HD12	1.88	0.56
1:B:88:GLU:OE1	1:B:88:GLU:N	2.34	0.56
1:B:397:GLU:HB3	1:B:411:ILE:HD12	1.87	0.55
1:B:29:ASN:OD1	1:B:33:LEU:HD21	2.06	0.55
1:A:397:GLU:HB3	1:A:411:ILE:HD12	1.88	0.54
2:C:18:VAL:CG2	2:C:297:VAL:HG12	2.37	0.54
1:B:41:ASP:OD1	1:B:43:LEU:HD22	2.08	0.54
2:D:405:PRO:HB3	2:D:411:ILE:HD13	1.90	0.53
1:B:292:ASP:OD2	1:B:457:ARG:NH1	2.38	0.53
1:B:356:LEU:O	1:B:357:ASN:CB	2.56	0.53
2:D:356:LEU:O	2:D:357:ASN:C	2.47	0.53
1:A:333:THR:OG1	1:A:334:PRO:HD3	2.09	0.53
1:B:333:THR:OG1	1:B:334:PRO:HD3	2.09	0.53
2:C:297:VAL:HG23	2:C:298:THR:HG23	1.90	0.53
2:D:18:VAL:CG2	2:D:297:VAL:HG12	2.39	0.53
1:B:321:GLU:HG2	1:B:417:ALA:HA	1.91	0.52
2:D:206:GLY:HA2	5:D:727:HOH:O	2.07	0.52
2:D:321:GLU:HG2	2:D:417:ALA:HA	1.91	0.52
1:B:75:TYR:HB2	1:B:92:VAL:CG2	2.39	0.52
2:C:333:THR:OG1	2:C:334:PRO:HD3	2.09	0.52
1:B:377:ALA:HB3	1:B:382:LYS:HE3	1.92	0.52
2:C:509:GLY:HA2	2:C:511:HIS:CE1	2.45	0.52
2:D:206:GLY:N	5:D:701:HOH:O	2.42	0.52
2:C:321:GLU:HG2	2:C:417:ALA:HA	1.92	0.52
1:B:49:ILE:HG12	1:B:85:TRP:HB2	1.92	0.52
2:D:297:VAL:HG23	2:D:298:THR:HG23	1.93	0.51
1:A:165:PRO:HB2	2:C:465:PHE:CD1	2.45	0.51
1:B:17:LYS:CE	1:B:57:LEU:HD13	2.41	0.51
2:D:333:THR:OG1	2:D:334:PRO:HD3	2.10	0.51
1:A:165:PRO:HB2	2:C:465:PHE:CG	2.46	0.51
1:A:321:GLU:HG2	1:A:417:ALA:HA	1.93	0.51
2:D:194:THR:O	2:D:198:ILE:HG13	2.11	0.51
1:A:49:ILE:HG12	1:A:85:TRP:HB2	1.93	0.50
1:B:17:LYS:CE	1:B:57:LEU:CD1	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:THR:O	1:B:198:ILE:HG13	2.12	0.50
2:D:66:ILE:HD13	2:D:91:VAL:HG12	1.91	0.50
1:A:18:VAL:CG2	1:A:297:VAL:HG12	2.42	0.49
1:B:41:ASP:OD1	1:B:43:LEU:CD2	2.59	0.49
1:B:60:ILE:HG13	1:B:80:ILE:HB	1.93	0.49
2:C:49:ILE:HG12	2:C:85:TRP:HB2	1.95	0.49
1:A:14:PHE:HB2	1:A:28:VAL:CG2	2.42	0.49
2:D:14:PHE:HB2	2:D:28:VAL:CG2	2.43	0.49
1:A:500:LYS:HA	2:C:508:TRP:CZ3	2.48	0.49
1:B:58:LEU:C	1:B:58:LEU:HD12	2.32	0.49
1:A:118:TYR:CE1	2:C:165:PRO:HG3	2.48	0.48
1:B:39:PHE:HE2	1:B:45:LEU:HD11	1.78	0.48
2:D:49:ILE:HG12	2:D:85:TRP:HB2	1.94	0.48
1:B:297:VAL:HG23	1:B:298:THR:HG23	1.96	0.48
1:B:45:LEU:N	1:B:45:LEU:HD12	2.28	0.48
1:A:331:LEU:CD1	1:A:384:LEU:CD2	2.91	0.48
1:B:18:VAL:CG2	1:B:297:VAL:HG12	2.43	0.47
1:B:39:PHE:CE2	1:B:45:LEU:HD11	2.49	0.47
1:B:331:LEU:CD1	1:B:384:LEU:CD2	2.92	0.47
1:A:509:GLY:HA2	1:A:511:HIS:CE1	2.49	0.47
1:B:17:LYS:HE2	1:B:57:LEU:CD1	2.45	0.47
1:B:27:ILE:HD12	1:B:49:ILE:HB	1.95	0.47
2:C:18:VAL:HG22	2:C:297:VAL:HG12	1.96	0.47
2:C:194:THR:O	2:C:198:ILE:HG13	2.13	0.47
2:D:58:LEU:HD12	2:D:58:LEU:N	2.30	0.47
2:C:23:ASN:HB2	2:C:58:LEU:HD21	1.96	0.46
1:A:194:THR:O	1:A:198:ILE:HG13	2.14	0.46
1:B:14:PHE:HB2	1:B:28:VAL:CG2	2.45	0.46
1:B:329:ILE:CG2	1:B:349:MSE:SE	3.13	0.46
2:D:331:LEU:CD1	2:D:384:LEU:CD2	2.94	0.46
1:B:124:ARG:HD2	1:B:130:VAL:HG22	1.97	0.46
1:B:397:GLU:OE2	1:B:406:THR:HG22	2.16	0.46
1:A:112:LEU:N	1:A:112:LEU:CD1	2.79	0.46
2:D:45:LEU:HD12	2:D:45:LEU:N	2.30	0.46
1:B:26:ILE:HG13	1:B:68:ARG:NH2	2.32	0.45
2:C:508:TRP:CE3	2:D:252:GLN:NE2	2.85	0.45
2:D:14:PHE:HB2	2:D:28:VAL:HG22	1.99	0.45
2:D:24:VAL:CA	2:D:57:LEU:HD13	2.47	0.44
1:A:14:PHE:HB2	1:A:28:VAL:HG22	1.98	0.44
1:A:297:VAL:HG23	1:A:298:THR:HG23	1.98	0.44
1:B:356:LEU:O	1:B:357:ASN:CG	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:405:PRO:HB3	2:D:411:ILE:CD1	2.46	0.44
1:A:99:LEU:N	1:A:99:LEU:CD1	2.81	0.44
2:D:166[B]:ASN:ND2	2:D:272:ARG:O	2.50	0.44
1:A:508:TRP:O	1:B:151:TYR:HE1	2.01	0.44
2:D:318:MSE:CE	2:D:426:GLN:HG2	2.48	0.43
1:A:348:GLU:CG	1:A:414:ALA:CB	2.96	0.43
1:A:109:PRO:HG3	1:A:392:LYS:O	2.18	0.43
1:B:109:PRO:HG2	1:B:392:LYS:O	2.18	0.43
2:D:213:LEU:HD12	2:D:254:MSE:HE1	2.01	0.43
2:D:24:VAL:HG13	2:D:54:LYS:HB2	1.99	0.43
1:B:87:ASP:OD1	1:B:88:GLU:OE1	2.37	0.43
1:A:331:LEU:HD12	1:A:384:LEU:CD2	2.48	0.43
1:B:136:LEU:HD21	1:B:209:MSE:CE	2.49	0.42
2:D:99:LEU:N	2:D:99:LEU:CD1	2.81	0.42
1:A:329:ILE:HD11	1:A:345:LEU:HG	2.01	0.42
2:D:109:PRO:HG3	2:D:392:LYS:O	2.19	0.42
2:C:123:TYR:HB3	2:C:272:ARG:NH2	2.35	0.42
2:D:294:PHE:HA	2:D:297:VAL:HG22	2.00	0.42
1:B:14:PHE:HB2	1:B:28:VAL:HG22	2.02	0.42
2:D:57:LEU:N	2:D:57:LEU:HD12	2.35	0.42
2:D:195:ILE:HD11	2:D:516:VAL:HG21	2.02	0.42
1:B:87:ASP:OD1	1:B:88:GLU:N	2.52	0.42
1:B:356:LEU:O	1:B:357:ASN:HB3	2.20	0.42
2:C:23:ASN:CB	2:C:58:LEU:HD21	2.50	0.42
2:C:294:PHE:HA	2:C:297:VAL:HG22	2.01	0.42
1:A:308:ASP:OD2	1:A:392:LYS:HG2	2.19	0.41
2:D:24:VAL:HA	2:D:57:LEU:HD13	2.02	0.41
1:A:136:LEU:HD21	1:A:209:MSE:CE	2.51	0.41
1:A:294:PHE:HA	1:A:297:VAL:HG22	2.02	0.41
2:C:136:LEU:HD21	2:C:209:MSE:CE	2.51	0.41
1:B:99:LEU:CD2	1:B:329:ILE:CD1	2.98	0.41
1:B:292:ASP:OD1	1:B:293:ALA:N	2.54	0.41
2:C:109:PRO:HG3	2:C:392:LYS:O	2.21	0.41
2:D:102:LEU:O	2:D:104:LEU:HD12	2.20	0.41
1:A:261:ILE:HD12	1:A:264:ARG:HH22	1.85	0.41
2:D:213:LEU:HA	2:D:254:MSE:SE	2.71	0.41
1:A:124:ARG:HD3	1:A:130:VAL:HG22	2.02	0.41
2:C:505:SER:HA	2:C:510:LEU:HD12	2.02	0.41
1:B:41:ASP:CG	1:B:43:LEU:HD22	2.41	0.41
1:A:333:THR:N	1:A:334:PRO:CD	2.84	0.41
1:A:292:ASP:OD1	1:A:293:ALA:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:380:VAL:O	2:C:384:LEU:HG	2.22	0.40
1:B:195:ILE:HD11	1:B:516:VAL:HG21	2.04	0.40
1:B:333:THR:N	1:B:334:PRO:CD	2.85	0.40
1:B:380:VAL:O	1:B:384:LEU:HG	2.21	0.40
2:C:333:THR:N	2:C:334:PRO:CD	2.84	0.40
1:A:112:LEU:HD12	1:A:112:LEU:H	1.87	0.40
2:D:380:VAL:O	2:D:384:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	452/526 (86%)	430 (95%)	22 (5%)	0	100	100
1	B	442/526 (84%)	425 (96%)	17 (4%)	0	100	100
2	C	445/526 (85%)	425 (96%)	20 (4%)	0	100	100
2	D	445/526 (85%)	425 (96%)	20 (4%)	0	100	100
All	All	1784/2104 (85%)	1705 (96%)	79 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/420 (90%)	375 (100%)	1 (0%)	92	95
1	B	372/420 (89%)	371 (100%)	1 (0%)	92	95
2	C	374/421 (89%)	374 (100%)	0	100	100
2	D	373/421 (89%)	373 (100%)	0	100	100
All	All	1495/1682 (89%)	1493 (100%)	2 (0%)	93	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	512	ASN
1	B	150	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	A	512	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	PHD	B	168	1	9,11,12	1.12	1 (11%)	10,15,17	0.66	0
1	PHD	A	168	1	9,11,12	1.33	1 (11%)	10,15,17	0.70	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
1	PHD	B	168	1	-	1/8/11/13	-
1	PHD	A	168	1	-	1/8/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	PHD	P-OD1	3.46	1.64	1.59
1	B	168	PHD	P-OD1	2.86	1.63	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	168	PHD	O-C-CA-CB
1	B	168	PHD	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	450/526 (85%)	-0.08	14 (3%)	49 58	33, 64, 112, 171	0
1	B	441/526 (83%)	0.18	16 (3%)	42 51	42, 81, 146, 178	0
2	C	444/526 (84%)	-0.14	10 (2%)	60 69	30, 61, 101, 162	0
2	D	443/526 (84%)	0.23	29 (6%)	18 22	38, 73, 183, 208	0
All	All	1778/2104 (84%)	0.05	69 (3%)	39 46	30, 68, 149, 208	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	46	ILE	7.9
1	B	15	TYR	7.2
2	C	143	HIS	6.9
1	B	14	PHE	6.9
2	D	40	PRO	6.4
2	D	67	ILE	5.7
1	B	45	LEU	5.4
2	D	84	SER	5.3
1	A	248	HIS	5.2
2	C	248	HIS	5.2
2	D	56	ALA	5.1
1	A	10	THR	5.1
1	B	186	PRO	5.1
1	A	143	HIS	4.7
1	A	180	GLY	4.6
2	D	248	HIS	4.4
1	A	247	LYS	4.2
2	D	77	VAL	4.1
2	D	57	LEU	4.0
2	D	186	PRO	4.0
2	D	14	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	11	PRO	3.8
2	C	377	ALA	3.7
2	D	39	PHE	3.7
1	A	376	LEU	3.6
1	A	186	PRO	3.5
2	D	41	ASP	3.5
2	D	143	HIS	3.4
1	B	212	GLY	3.4
1	A	187	ALA	3.4
2	D	76	ALA	3.4
2	D	78	ARG	3.4
2	C	246	GLU	3.3
2	C	10	THR	3.3
2	D	46	ILE	3.3
2	D	52	GLY	3.2
1	B	117	GLY	3.0
2	D	12	THR	3.0
1	B	143	HIS	2.9
1	A	185	ALA	2.9
1	B	49	ILE	2.9
1	B	99	LEU	2.9
2	D	15	TYR	2.8
1	B	245	ASP	2.7
2	D	35	ALA	2.6
2	D	28	VAL	2.6
1	A	179	CYS	2.6
2	C	110	GLU	2.6
2	C	142	VAL	2.6
1	B	337	VAL	2.6
2	C	247	LYS	2.5
1	A	12	THR	2.5
2	D	82	ARG	2.5
2	D	85	TRP	2.4
2	D	74	GLY	2.4
1	A	178	GLY	2.3
1	B	93	LEU	2.3
2	C	187	ALA	2.3
2	D	75	TYR	2.2
1	A	377	ALA	2.2
2	D	117	GLY	2.2
2	D	38	ARG	2.2
1	B	177	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	72	VAL	2.2
1	B	304	GLY	2.1
2	D	185	ALA	2.1
2	D	95	GLU	2.1
1	B	142	VAL	2.1
2	C	196	HIS	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	PHD	B	168	12/13	0.89	0.16	61,73,90,91	4
1	PHD	A	168	12/13	0.90	0.14	46,56,92,93	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	CA	A	602	1/1	0.69	0.15	92,92,92,92	0
4	CL	D	604	1/1	0.69	0.17	97,97,97,97	0
4	CL	A	606	1/1	0.73	0.20	88,88,88,88	0
4	CL	D	605	1/1	0.80	0.12	89,89,89,89	0
3	CA	D	602	1/1	0.83	0.24	102,102,102,102	0
4	CL	D	603	1/1	0.85	0.19	85,85,85,85	0
4	CL	A	605	1/1	0.87	0.13	76,76,76,76	0
3	CA	C	602	1/1	0.88	0.10	99,99,99,99	0
3	CA	B	602	1/1	0.89	0.07	104,104,104,104	0
4	CL	A	604	1/1	0.91	0.26	86,86,86,86	0

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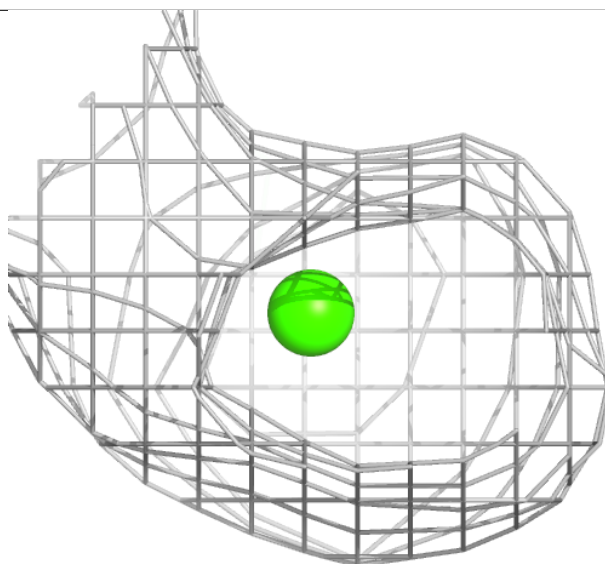
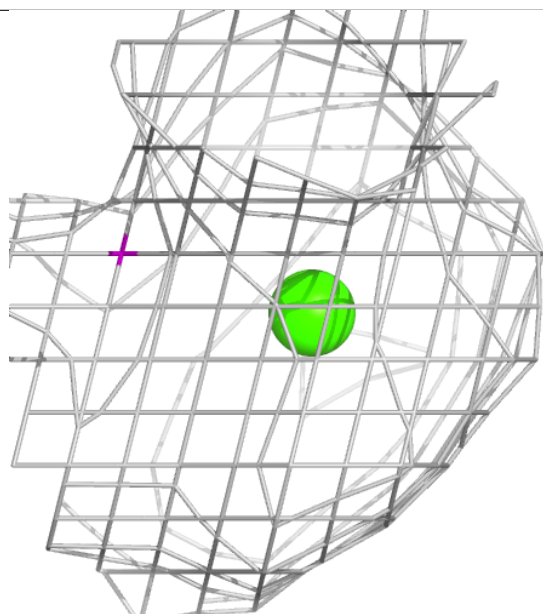
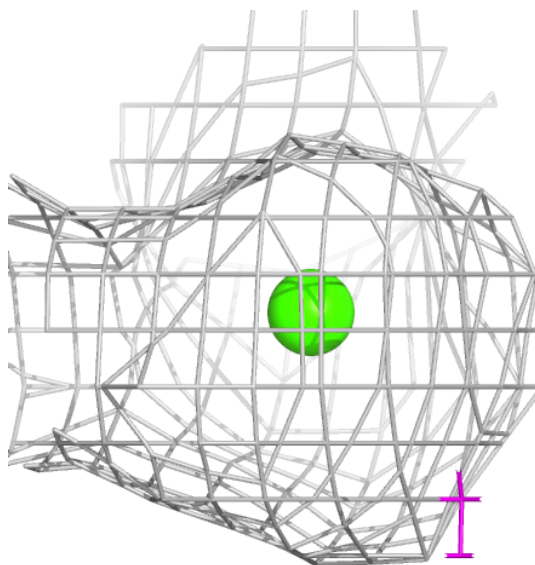
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	A	603	1/1	0.92	0.11	63,63,63,63	1
3	CA	C	601	1/1	0.93	0.06	51,51,51,51	0
3	CA	A	601	1/1	0.94	0.06	62,62,62,62	0
3	CA	D	601	1/1	0.95	0.08	65,65,65,65	0
4	CL	A	607	1/1	0.96	0.38	77,77,77,77	0
3	CA	B	601	1/1	0.96	0.10	69,69,69,69	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.

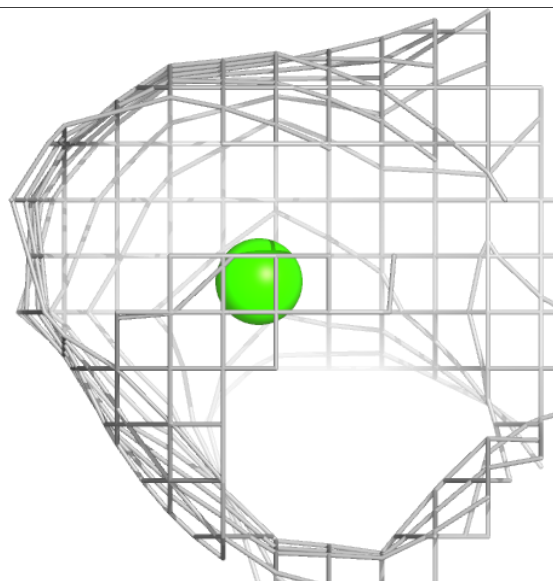
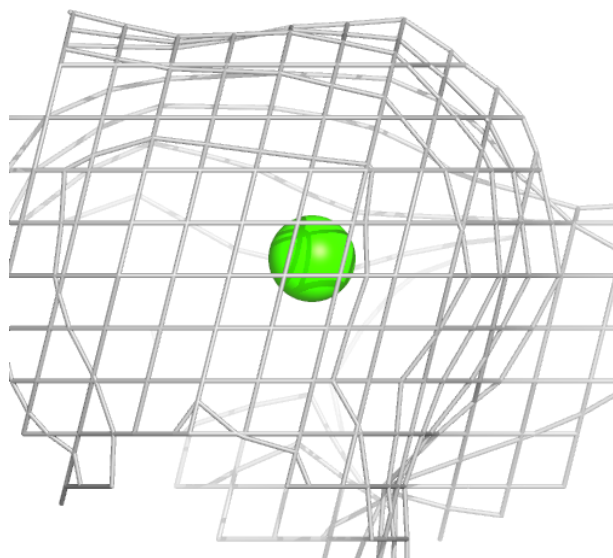
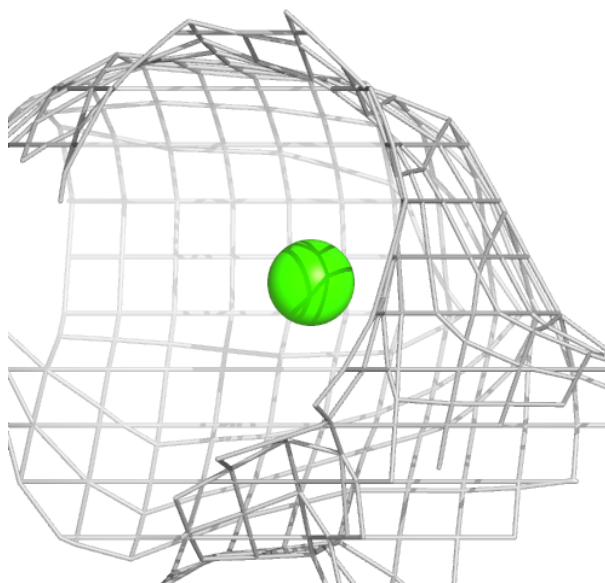
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



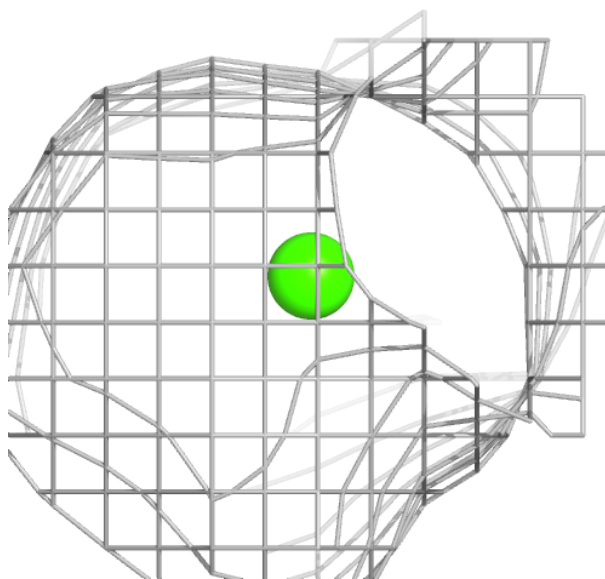
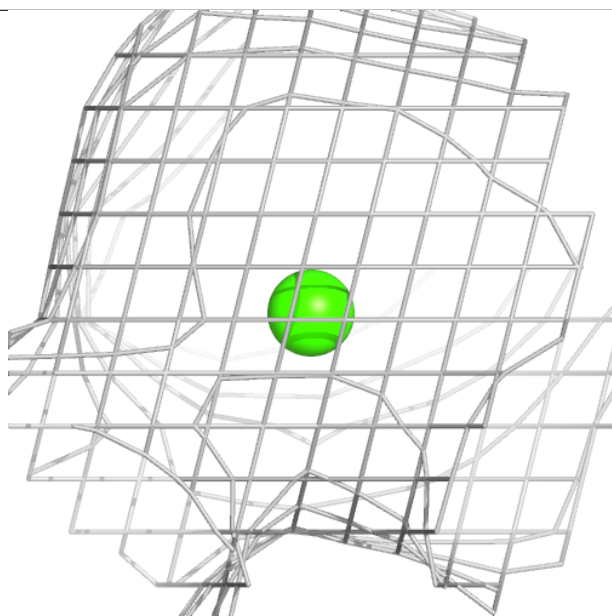
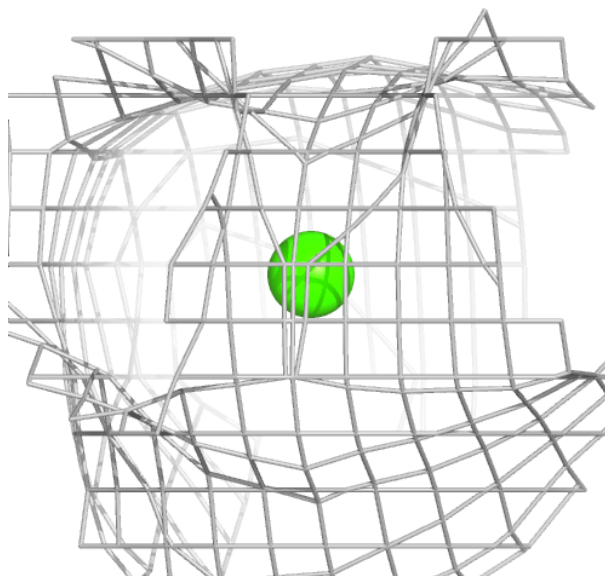
**Electron density around CA D 602:**

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



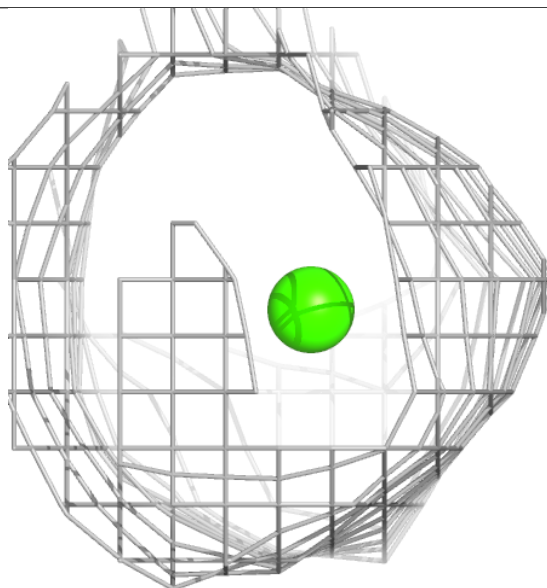
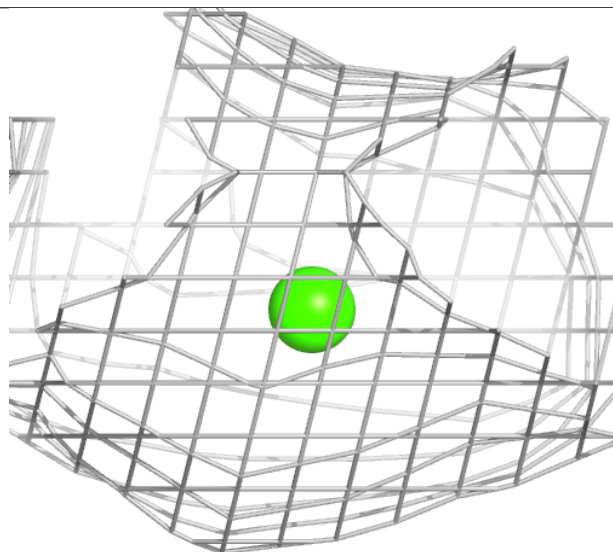
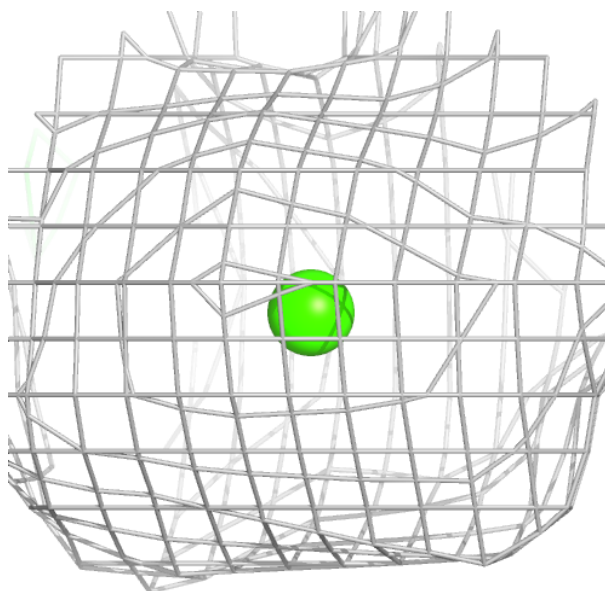
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and green (positive)



**Electron density around CA B 602:**

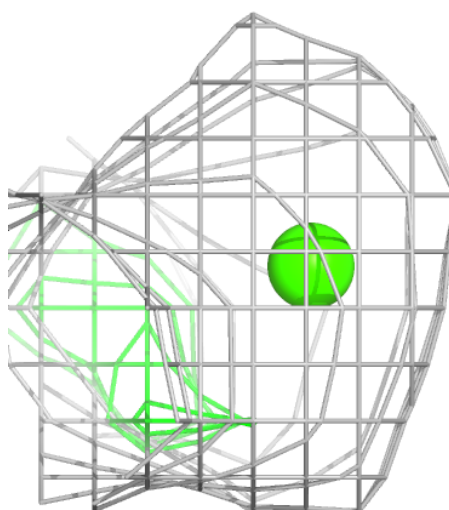
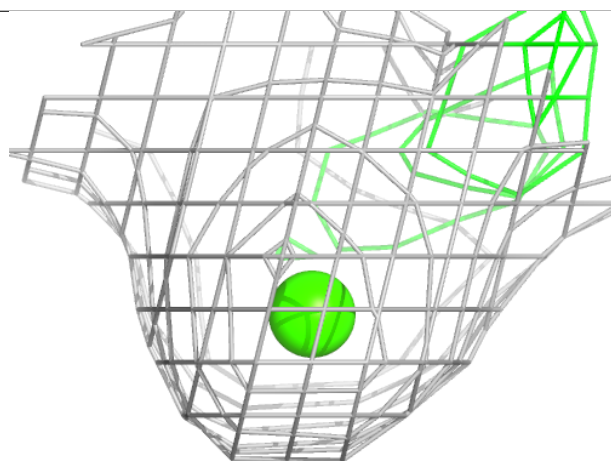
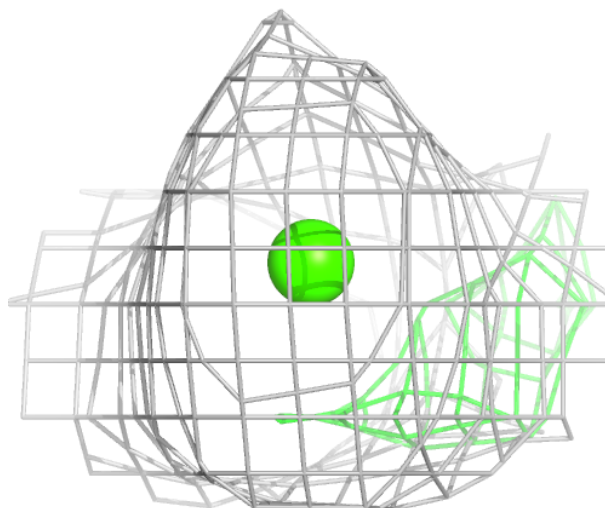
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and green (positive)





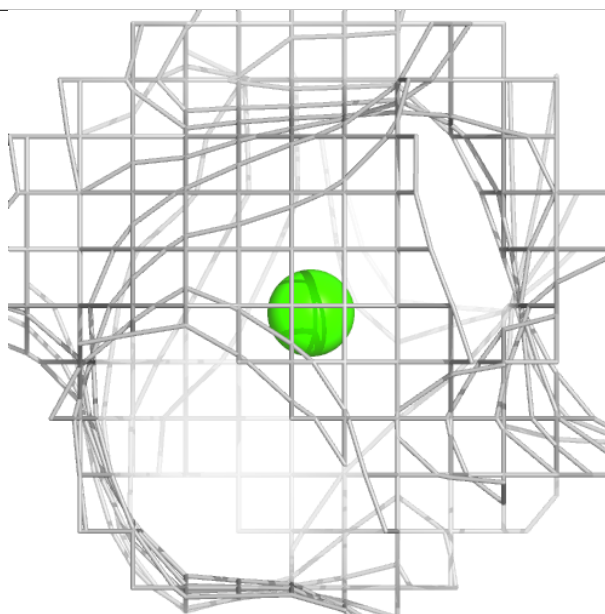
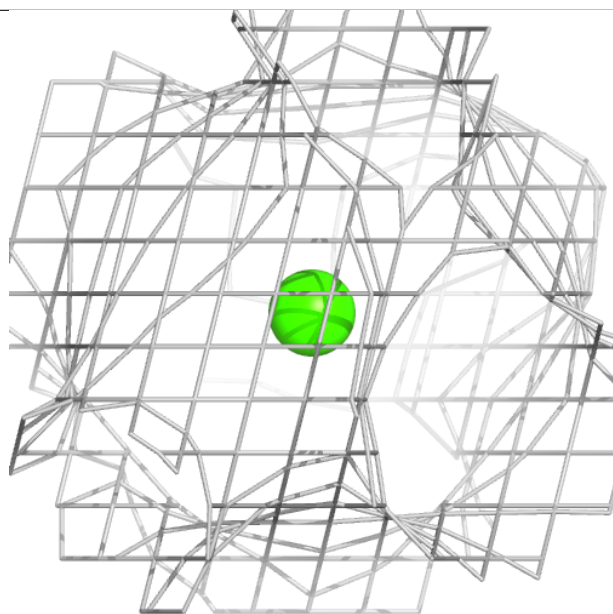
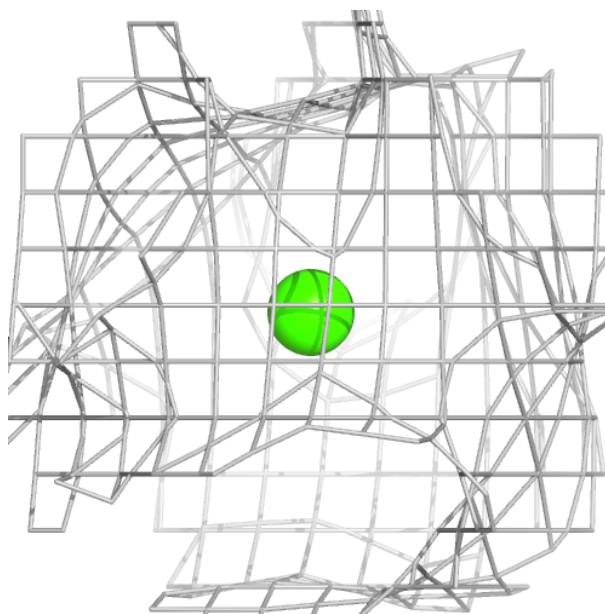
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and green (positive)



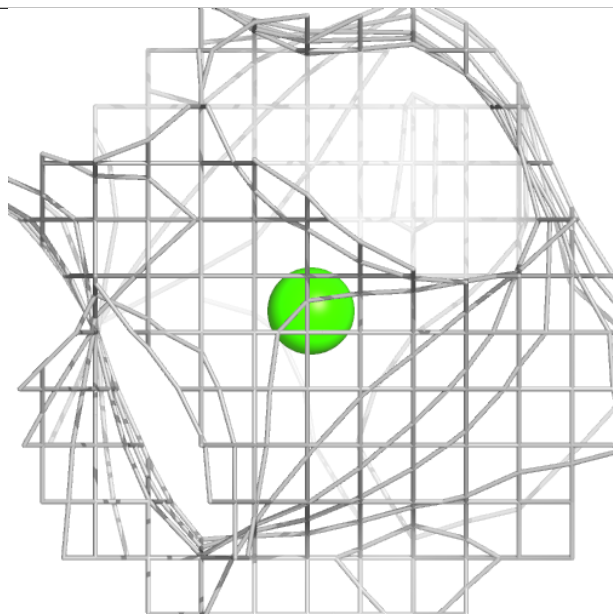
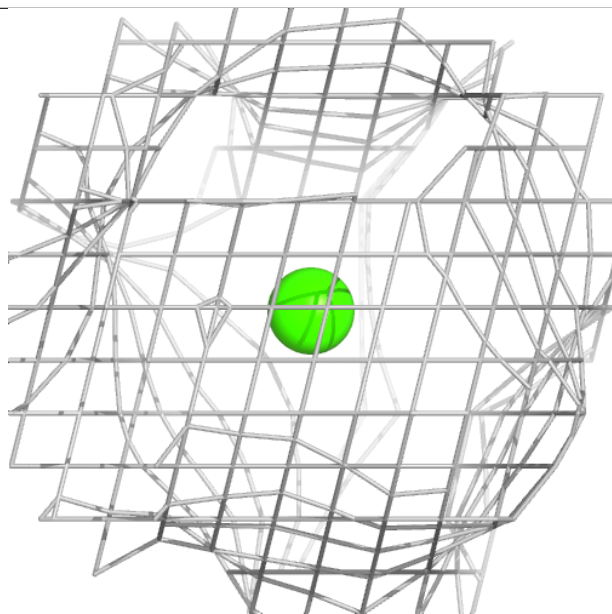
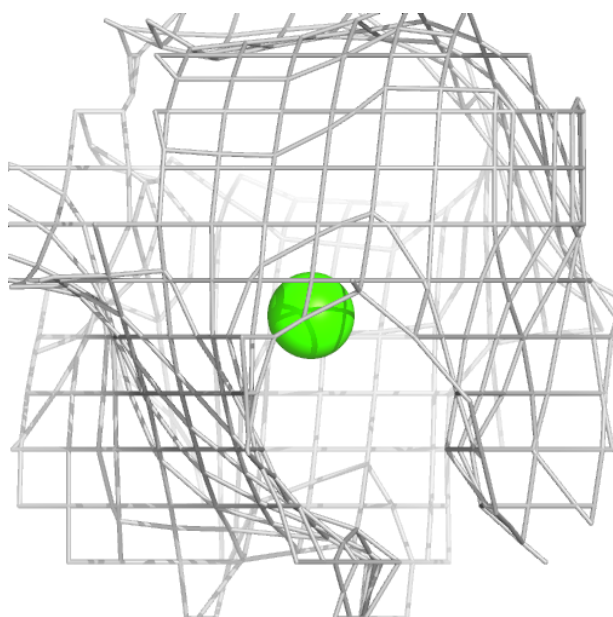
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and green (positive)



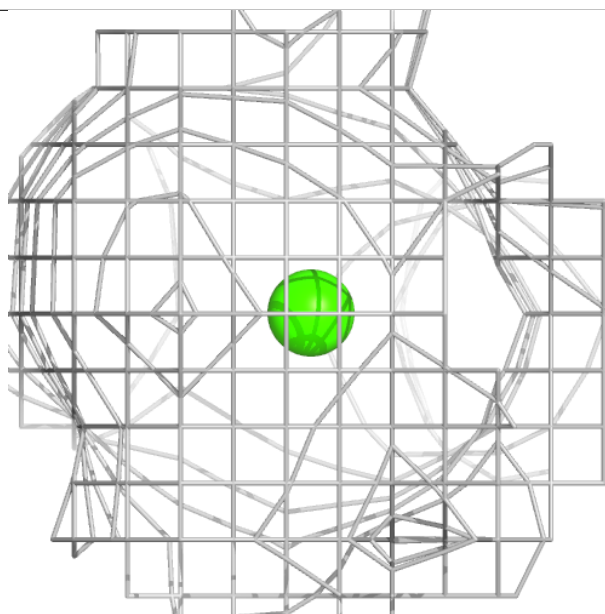
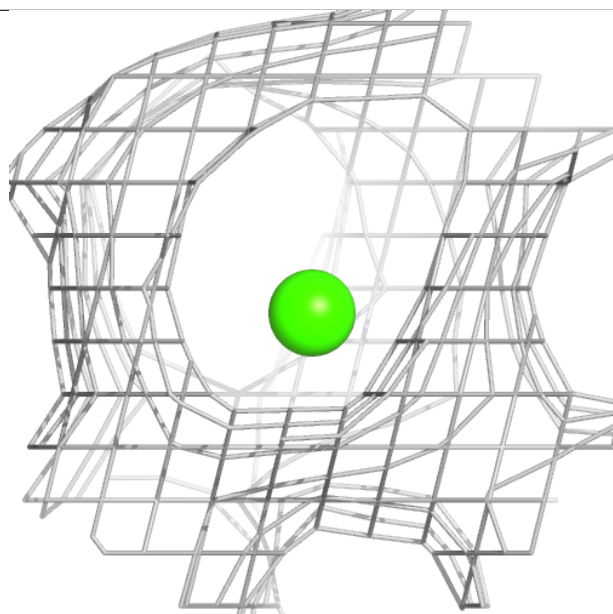
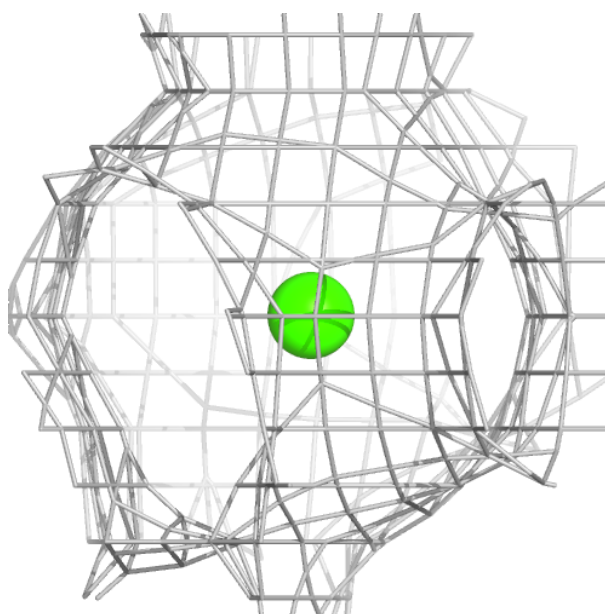
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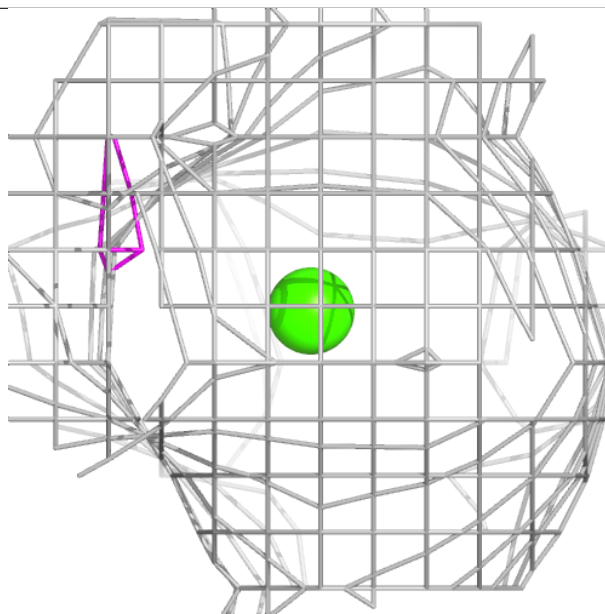
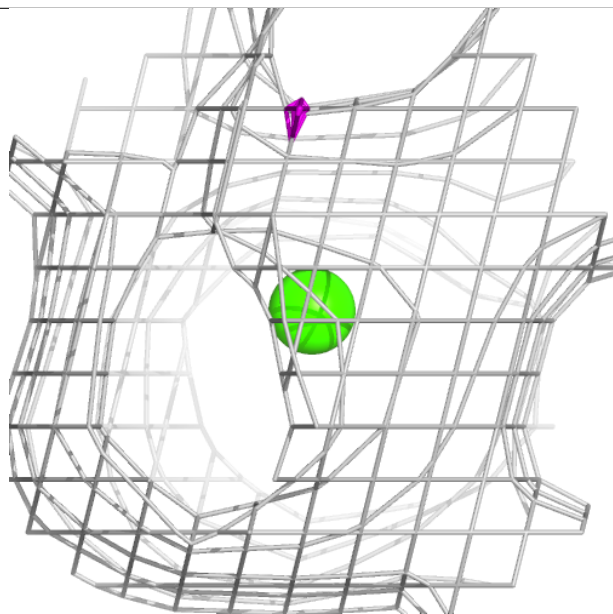
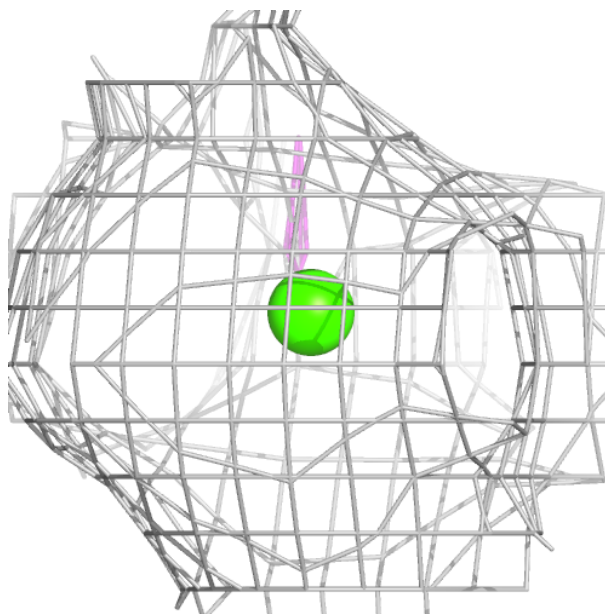
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and green (positive)



**Electron density around CA B 601:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.