



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2023 – 06:08 PM EDT

PDB ID : 8TXN
Title : Adaptive mechanism of collagen IV scaffold assembly in Drosophila: crystal structure of recombinant NC1 hexamer
Authors : Boudko, S.P.
Deposited on : 2023-08-23
Resolution : 1.75 Å(reported)

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

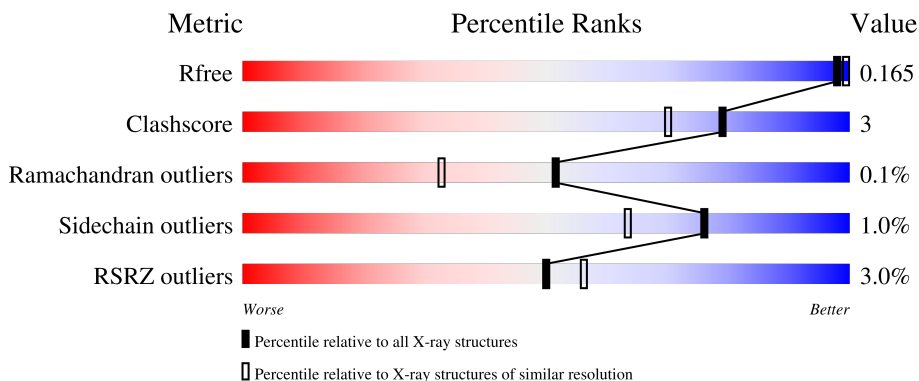
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	726	 2% 86% 7% 7%
1	D	726	 4% 87% 6% 7%

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
6	PEG	A	3009	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 11574 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 Collagen alpha-1(IV) chain, Collagen IV - chain Viking, Collagen alpha-1(IV) chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	674	5260	3281	917	1003	59	0	15	0
1	D	676	5296	3311	920	1005	60	0	15	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	ALA	-	expression tag	UNP P08120
A	-15	PRO	-	expression tag	UNP P08120
A	-14	LEU	-	expression tag	UNP P08120
A	-13	ALA	-	expression tag	UNP P08120
A	-12	ASP	-	expression tag	UNP P08120
A	-11	TYR	-	expression tag	UNP P08120
A	-10	LYS	-	expression tag	UNP P08120
A	-9	ASP	-	expression tag	UNP P08120
A	-8	ASP	-	expression tag	UNP P08120
A	-7	ASP	-	expression tag	UNP P08120
A	-6	ASP	-	expression tag	UNP P08120
A	-5	LYS	-	expression tag	UNP P08120
A	-4	LEU	-	expression tag	UNP P08120
A	-3	ALA	-	expression tag	UNP P08120
A	-2	SER	-	expression tag	UNP P08120
A	-1	THR	-	expression tag	UNP P08120
A	230	GLY	-	linker	UNP P08120
A	231	SER	-	linker	UNP P08120
A	232	SER	-	linker	UNP P08120
A	233	ALA	-	linker	UNP P08120
A	234	SER	-	linker	UNP P08120
A	235	SER	-	linker	UNP P08120
A	236	GLY	-	linker	UNP P08120
A	1230	GLY	-	linker	UNP Q9VMV5

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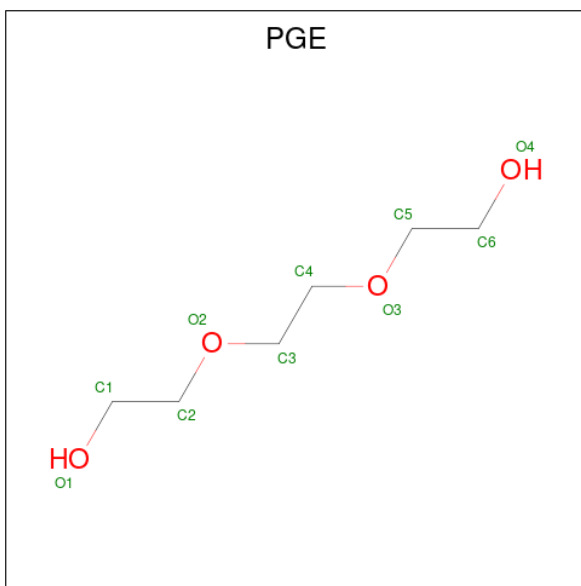
Chain	Residue	Modelled	Actual	Comment	Reference
A	1231	SER	-	linker	UNP Q9VMV5
A	1232	SER	-	linker	UNP Q9VMV5
A	1233	ALA	-	linker	UNP Q9VMV5
A	1234	SER	-	linker	UNP Q9VMV5
A	1235	SER	-	linker	UNP Q9VMV5
A	1236	GLY	-	linker	UNP Q9VMV5
A	2230	GLY	-	cloning artifact	UNP P08120
A	2231	SER	-	cloning artifact	UNP P08120
A	2232	GLY	-	cloning artifact	UNP P08120
A	2233	SER	-	cloning artifact	UNP P08120
A	2234	GLY	-	cloning artifact	UNP P08120
A	2235	SER	-	cloning artifact	UNP P08120
D	-16	ALA	-	expression tag	UNP P08120
D	-15	PRO	-	expression tag	UNP P08120
D	-14	LEU	-	expression tag	UNP P08120
D	-13	ALA	-	expression tag	UNP P08120
D	-12	ASP	-	expression tag	UNP P08120
D	-11	TYR	-	expression tag	UNP P08120
D	-10	LYS	-	expression tag	UNP P08120
D	-9	ASP	-	expression tag	UNP P08120
D	-8	ASP	-	expression tag	UNP P08120
D	-7	ASP	-	expression tag	UNP P08120
D	-6	ASP	-	expression tag	UNP P08120
D	-5	LYS	-	expression tag	UNP P08120
D	-4	LEU	-	expression tag	UNP P08120
D	-3	ALA	-	expression tag	UNP P08120
D	-2	SER	-	expression tag	UNP P08120
D	-1	THR	-	expression tag	UNP P08120
D	230	GLY	-	linker	UNP P08120
D	231	SER	-	linker	UNP P08120
D	232	SER	-	linker	UNP P08120
D	233	ALA	-	linker	UNP P08120
D	234	SER	-	linker	UNP P08120
D	235	SER	-	linker	UNP P08120
D	236	GLY	-	linker	UNP P08120
D	1230	GLY	-	linker	UNP Q9VMV5
D	1231	SER	-	linker	UNP Q9VMV5
D	1232	SER	-	linker	UNP Q9VMV5
D	1233	ALA	-	linker	UNP Q9VMV5
D	1234	SER	-	linker	UNP Q9VMV5
D	1235	SER	-	linker	UNP Q9VMV5
D	1236	GLY	-	linker	UNP Q9VMV5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2230	GLY	-	cloning artifact	UNP P08120
D	2231	SER	-	cloning artifact	UNP P08120
D	2232	GLY	-	cloning artifact	UNP P08120
D	2233	SER	-	cloning artifact	UNP P08120
D	2234	GLY	-	cloning artifact	UNP P08120
D	2235	SER	-	cloning artifact	UNP P08120

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 6 4	0	0
2	A	1	Total C O 10 6 4	0	0
2	A	1	Total C O 10 6 4	0	0
2	D	1	Total C O 10 6 4	0	0
2	D	1	Total C O 10 6 4	0	0

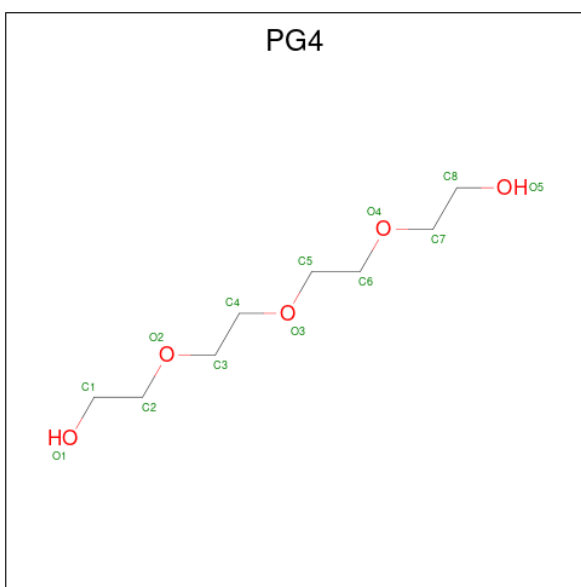
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



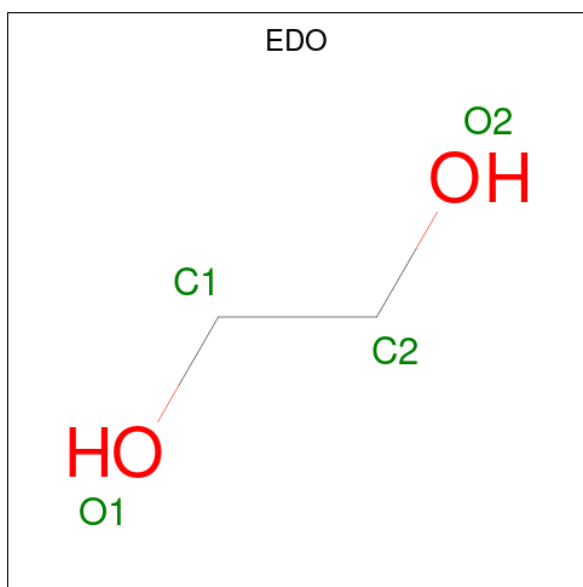
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 8 5	0	0
5	D	1	Total C O 13 8 5	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



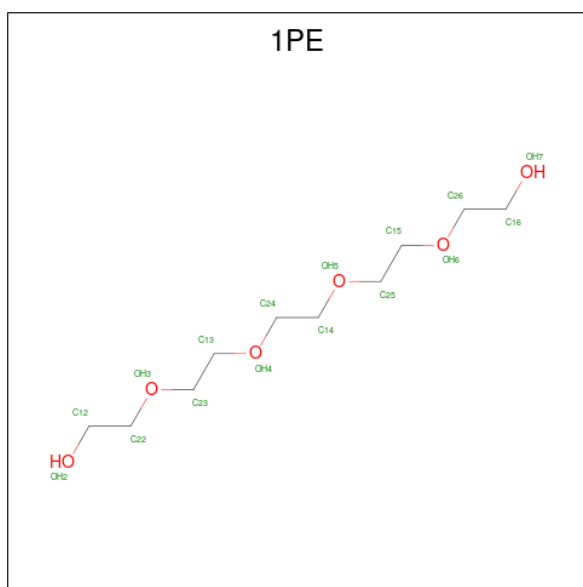
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		

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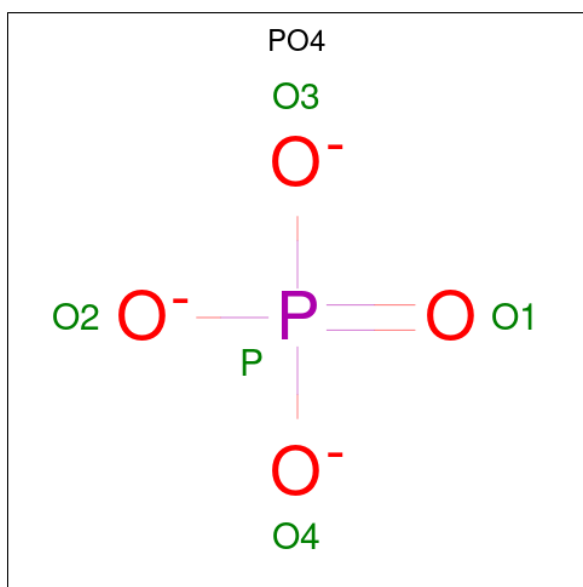
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			16	10	6		
8	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	O	P	0	0
			5	4	1		

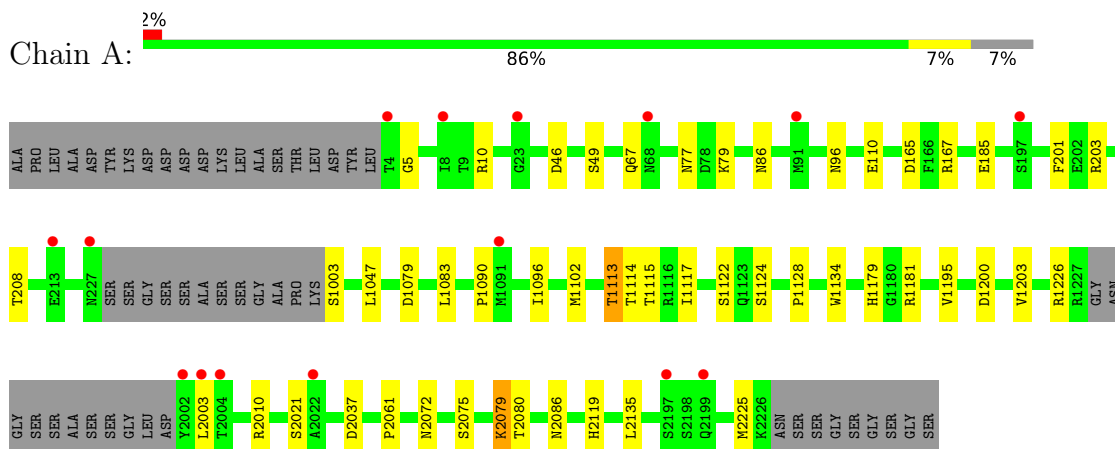
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	433	Total	O	0	0
			433	433		
10	D	429	Total	O	0	0
			429	429		

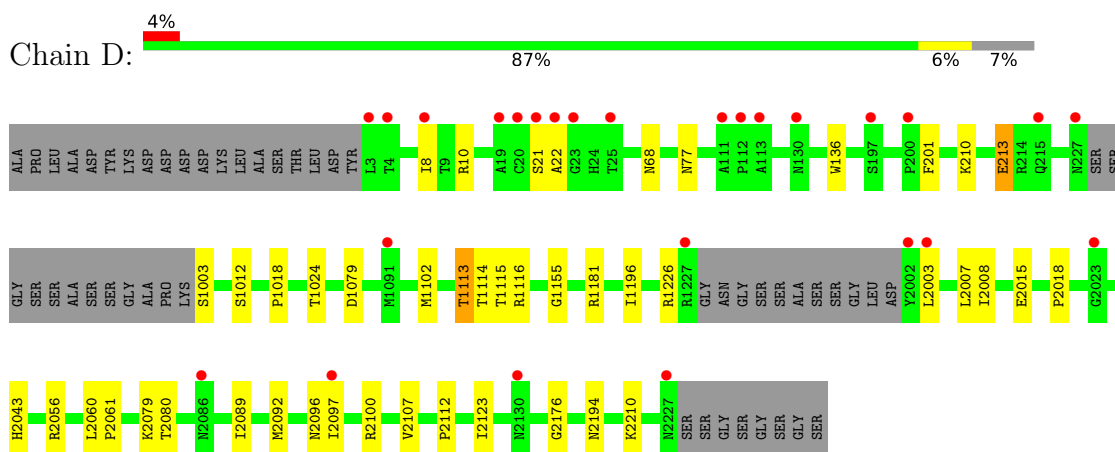
3 Residue-property plots [i](#)

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: Collagen alpha-1(IV) chain, Collagen IV - chain Viking, Collagen alpha-1(IV) chain



- Molecule 1: Collagen alpha-1(IV) chain, Collagen IV - chain Viking, Collagen alpha-1(IV) chain



4 Data and refinement statistics i

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	139.12Å 139.12Å 103.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.69 – 1.75 52.05 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (51.69-1.75) 98.5 (52.05-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.09 (at 1.75Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.142 , 0.164 0.142 , 0.165	Depositor DCC
R_{free} test set	2003 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtrriage
Anisotropy	0.310	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.031 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11574	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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: EDO, CL, 1PE, PO4, PG4, MG, PGE, PEG

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	0.35	0/5436	0.60	0/7397
1	D	0.35	0/5476	0.61	0/7451
All	All	0.35	0/10912	0.61	0/14848

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5260	0	4987	30	0
1	D	5296	0	5049	27	0
2	A	30	0	42	2	0
2	D	20	0	28	1	0
3	A	2	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	13	0	18	0	0
5	D	13	0	18	0	0
6	A	14	0	20	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	7	0	10	0	0
7	A	4	0	6	0	0
7	D	12	0	18	1	0
8	D	32	0	44	2	0
9	D	5	0	0	0	0
10	A	433	0	0	3	0
10	D	429	0	0	2	0
All	All	11574	0	10240	58	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 3.

The worst 5 of 58 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2119:HIS:H	6:A:3009:PEG:H32	1.43	0.84
1:A:77[B]:ASN:ND2	10:A:4001:HOH:O	2.21	0.74
1:D:10:ARG:NH2	1:D:21:SER:OG	2.21	0.73
1:D:2015:GLU:OE1	1:D:2100[B]:ARG:NH1	2.23	0.70
1:A:2119:HIS:N	6:A:3009:PEG:H32	2.06	0.68

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	683/726 (94%)	669 (98%)	13 (2%)	1 (0%)	51 33
1	D	686/726 (94%)	669 (98%)	16 (2%)	1 (0%)	51 33
All	All	1369/1452 (94%)	1338 (98%)	29 (2%)	2 (0%)	51 33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	22	ALA
1	A	96	ASN

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	589/618 (95%)	582 (99%)	7 (1%)	71	56
1	D	595/618 (96%)	590 (99%)	5 (1%)	81	72
All	All	1184/1236 (96%)	1172 (99%)	12 (1%)	76	63

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	213	GLU
1	D	1079	ASP
1	D	2079	LYS
1	D	1113	THR
1	A	1113	THR

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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	PGE	D	3007	-	9,9,9	0.51	0	8,8,8	0.38	0
6	PEG	D	3010	-	6,6,6	0.50	0	5,5,5	0.23	0
7	EDO	D	3009	-	3,3,3	0.46	0	2,2,2	0.34	0
5	PG4	A	3005	-	12,12,12	0.53	0	11,11,11	0.28	0
7	EDO	D	3012	-	3,3,3	0.49	0	2,2,2	0.32	0
8	1PE	D	3006	-	15,15,15	0.54	0	14,14,14	0.36	0
6	PEG	A	3007	-	6,6,6	0.48	0	5,5,5	0.26	0
2	PGE	D	3005	-	9,9,9	0.51	0	8,8,8	0.22	0
7	EDO	D	3011	-	3,3,3	0.48	0	2,2,2	0.36	0
2	PGE	A	3001	-	9,9,9	0.74	0	8,8,8	0.92	1 (12%)
2	PGE	A	3006	-	9,9,9	0.51	0	8,8,8	0.28	0
8	1PE	D	3008	-	15,15,15	0.54	0	14,14,14	0.33	0
5	PG4	D	3004	-	12,12,12	0.52	0	11,11,11	0.33	0
9	PO4	D	3013	-	4,4,4	1.06	0	6,6,6	0.56	0
7	EDO	A	3010	-	3,3,3	0.47	0	2,2,2	0.36	0
6	PEG	A	3009	-	6,6,6	0.52	0	5,5,5	0.60	0
2	PGE	A	3008	-	9,9,9	0.48	0	8,8,8	0.29	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
2	PGE	D	3007	-	-	4/7/7/7	-
6	PEG	D	3010	-	-	2/4/4/4	-
7	EDO	D	3009	-	-	1/1/1/1	-
5	PG4	A	3005	-	-	2/10/10/10	-
7	EDO	D	3012	-	-	0/1/1/1	-
8	1PE	D	3006	-	-	9/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	A	3007	-	-	3/4/4/4	-
2	PGE	D	3005	-	-	3/7/7/7	-
7	EDO	D	3011	-	-	0/1/1/1	-
2	PGE	A	3001	-	-	5/7/7/7	-
2	PGE	A	3006	-	-	4/7/7/7	-
8	1PE	D	3008	-	-	5/13/13/13	-
5	PG4	D	3004	-	-	5/10/10/10	-
7	EDO	A	3010	-	-	1/1/1/1	-
6	PEG	A	3009	-	-	2/4/4/4	-
2	PGE	A	3008	-	-	0/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	PGE	O3-C5-C6	2.15	119.53	110.07

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3007	PGE	C1-C2-O2-C3
6	A	3009	PEG	O2-C3-C4-O4
2	D	3005	PGE	O2-C3-C4-O3
8	D	3008	1PE	OH6-C15-C25-OH5
5	D	3004	PG4	O2-C3-C4-O3

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3007	PGE	1	0
7	D	3012	EDO	1	0
8	D	3006	1PE	1	0
2	A	3001	PGE	1	0
8	D	3008	1PE	1	0
6	A	3009	PEG	4	0
2	A	3008	PGE	1	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	A	674/726 (92%)	-0.29	15 (2%) 62 69	9, 19, 38, 64	0
1	D	676/726 (93%)	-0.03	26 (3%) 40 47	10, 21, 40, 64	0
All	All	1350/1452 (92%)	-0.16	41 (3%) 50 56	9, 20, 39, 64	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	22	ALA	7.7
1	D	23	GLY	6.4
1	A	2022	ALA	5.2
1	D	2002	TYR	4.4
1	D	3	LEU	4.2

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 monosaccharides in this entry.

6.4 Ligands [i](#)

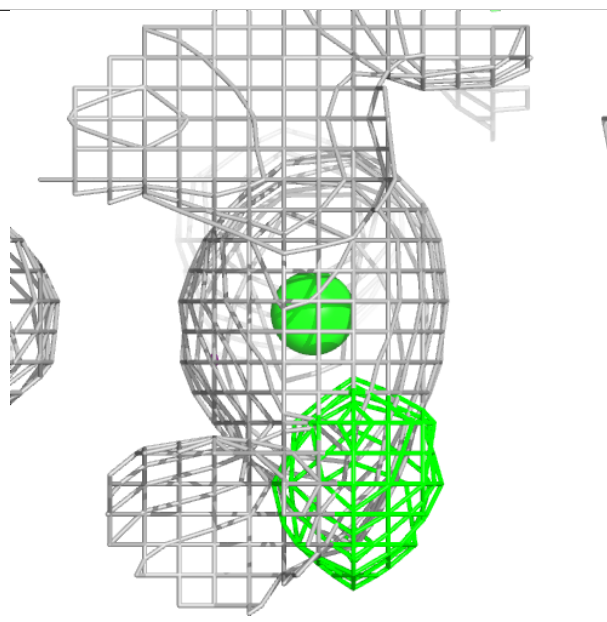
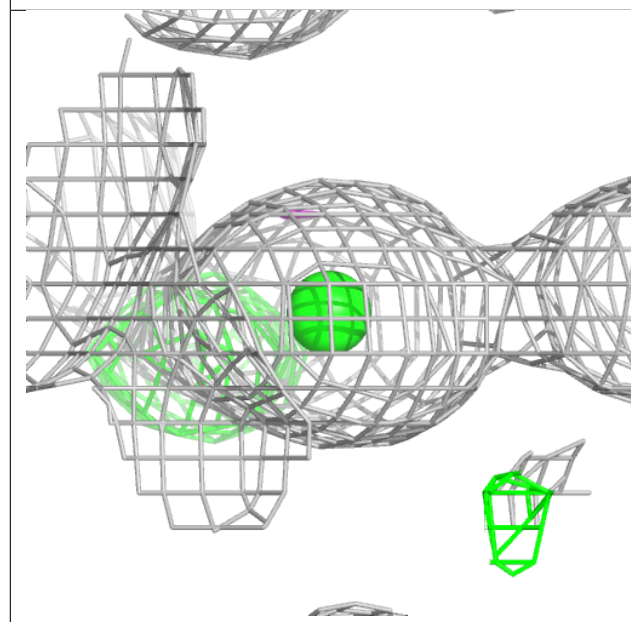
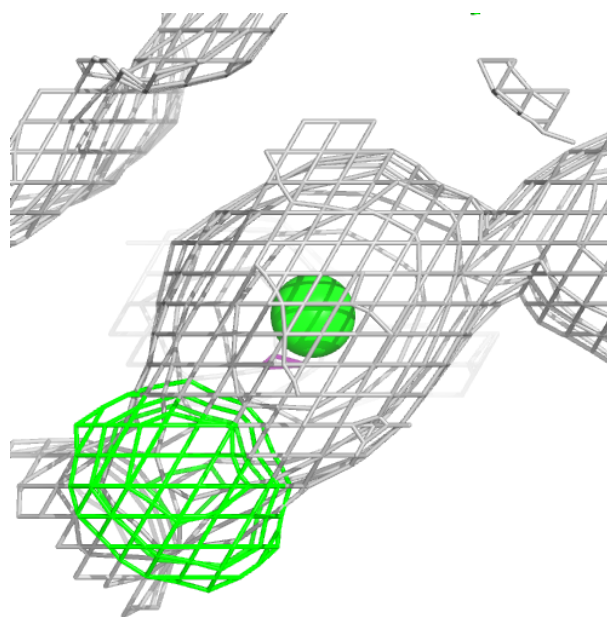
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PGE	D	3005	10/10	0.58	0.20	56,61,65,67	0
2	PGE	A	3006	10/10	0.70	0.21	54,59,66,70	0
7	EDO	D	3012	4/4	0.75	0.20	45,47,50,53	0
5	PG4	A	3005	13/13	0.76	0.20	43,49,55,56	0
2	PGE	D	3007	10/10	0.76	0.17	43,51,54,54	0
6	PEG	A	3007	7/7	0.77	0.17	46,49,55,61	0
6	PEG	D	3010	7/7	0.83	0.19	51,52,56,60	0
5	PG4	D	3004	13/13	0.84	0.20	34,37,43,44	0
8	1PE	D	3006	16/16	0.84	0.26	38,46,59,59	0
2	PGE	A	3001	10/10	0.85	0.12	37,44,48,51	0
7	EDO	A	3010	4/4	0.86	0.12	42,48,51,53	0
7	EDO	D	3011	4/4	0.86	0.10	53,54,54,54	0
8	1PE	D	3008	16/16	0.86	0.15	35,46,57,59	0
6	PEG	A	3009	7/7	0.87	0.27	24,28,32,45	0
7	EDO	D	3009	4/4	0.88	0.15	41,43,46,47	0
2	PGE	A	3008	10/10	0.95	0.13	31,32,41,51	0
3	CL	D	3002	1/1	0.98	0.05	28,28,28,28	0
9	PO4	D	3013	5/5	0.98	0.06	27,29,32,35	5
3	CL	A	3003	1/1	0.99	0.05	19,19,19,19	0
4	MG	A	3004	1/1	0.99	0.05	15,15,15,15	0
4	MG	D	3003	1/1	0.99	0.03	14,14,14,14	0
3	CL	D	3001	1/1	1.00	0.06	12,12,12,12	0
3	CL	A	3002	1/1	1.00	0.05	13,13,13,13	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.

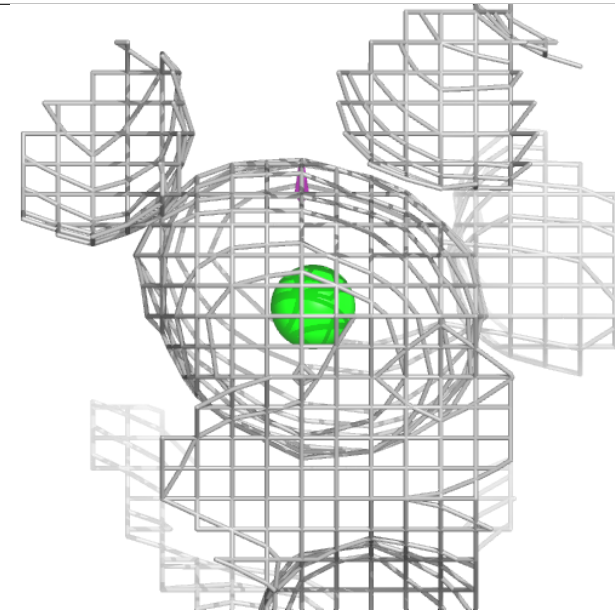
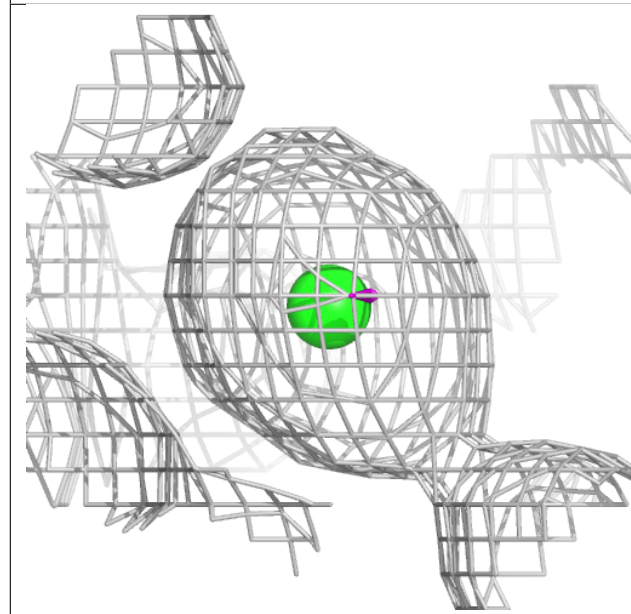
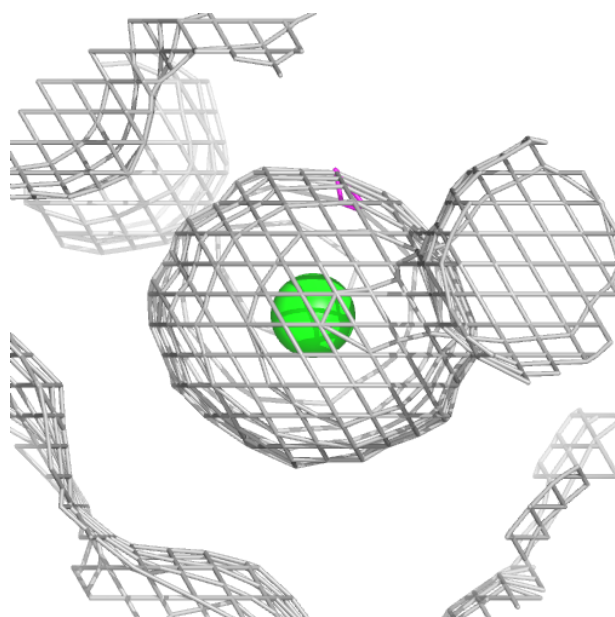
Electron density around CL D 3002:

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



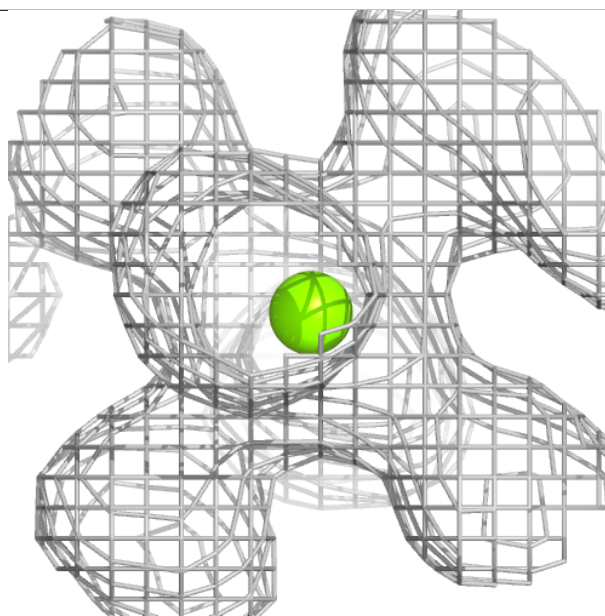
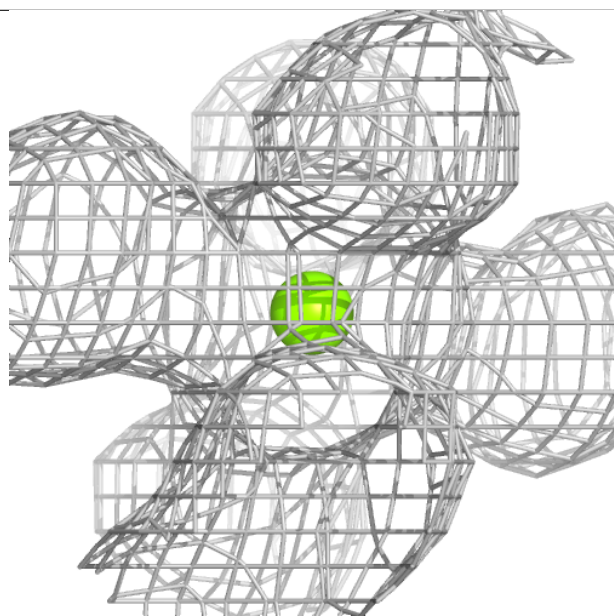
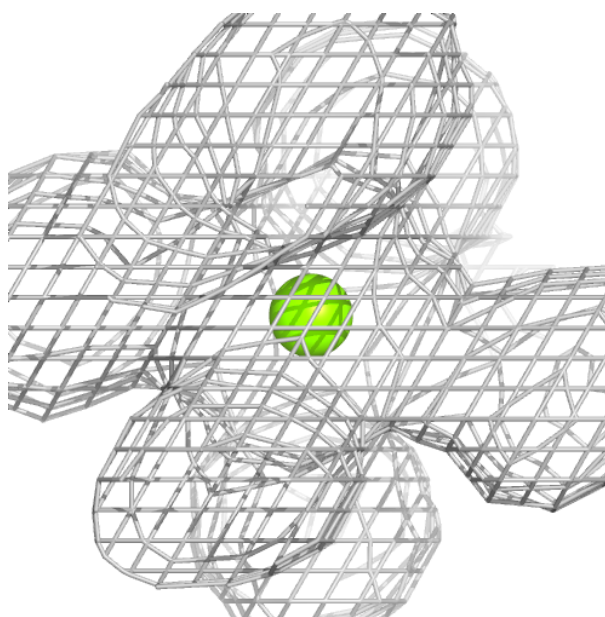
Electron density around CL A 3003:

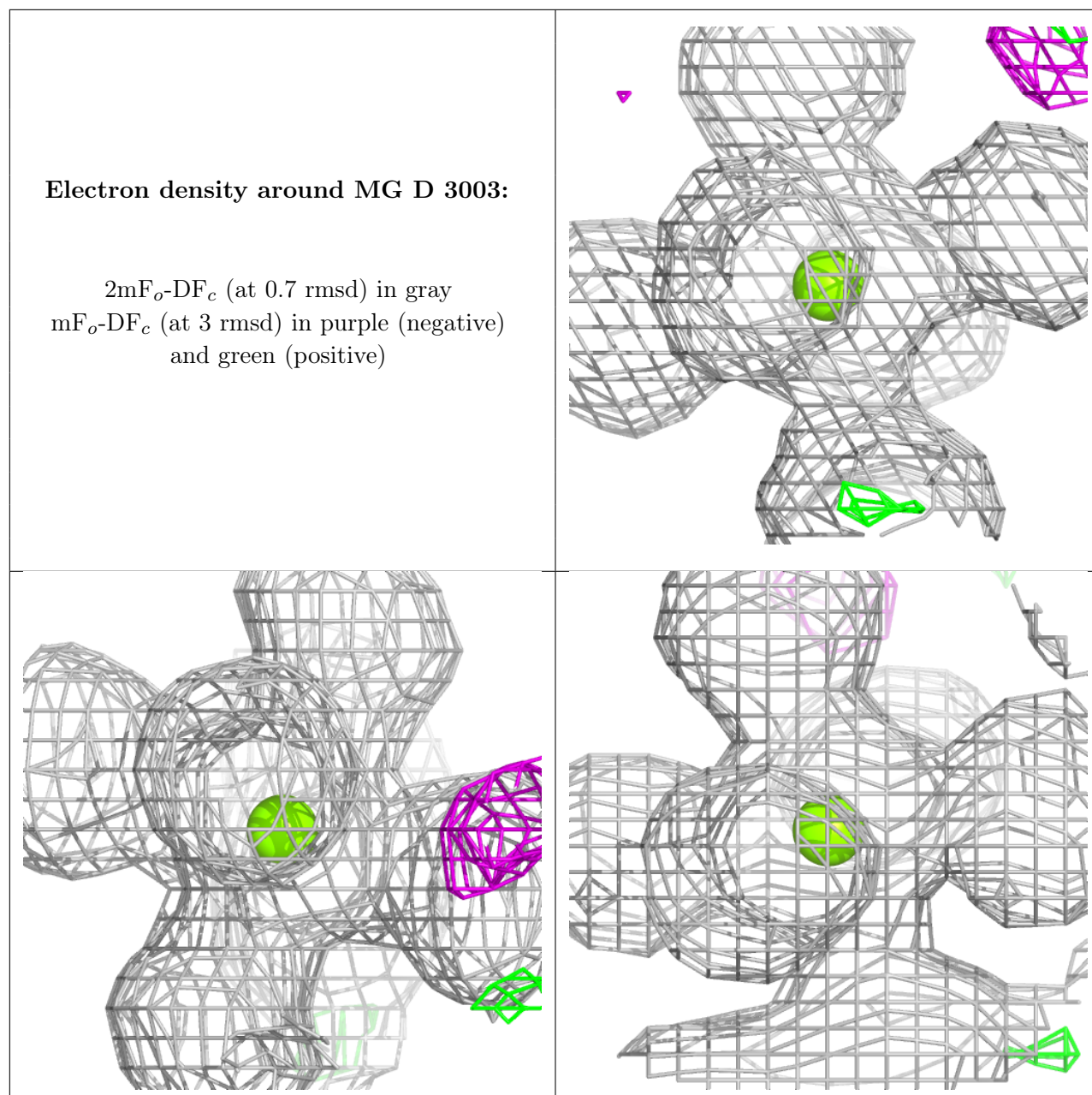
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG A 3004:

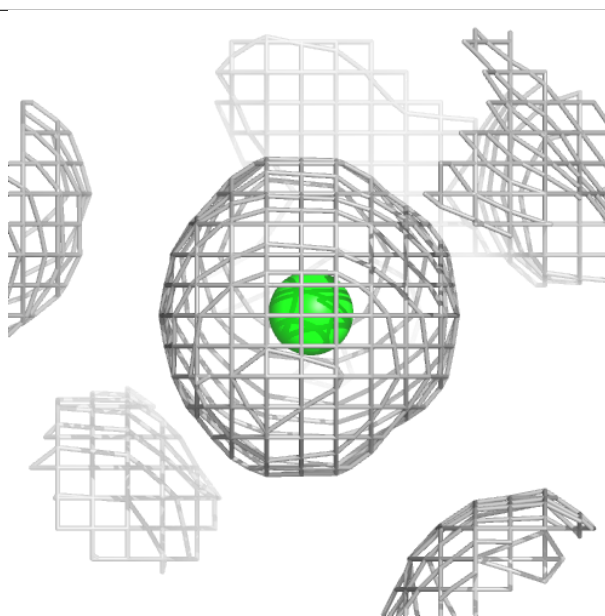
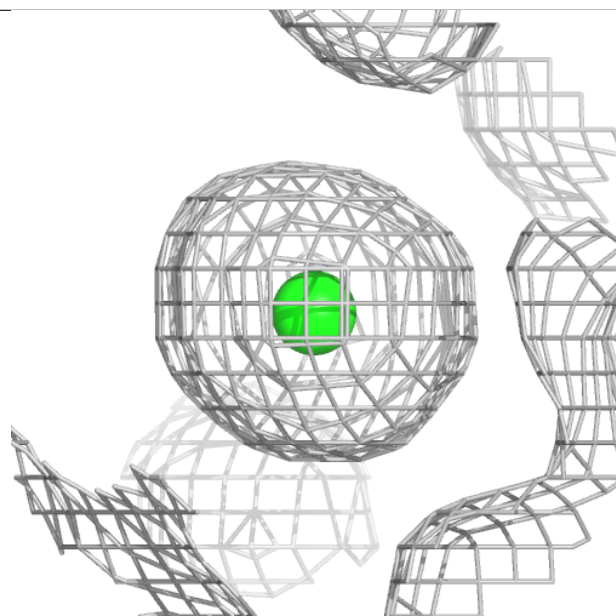
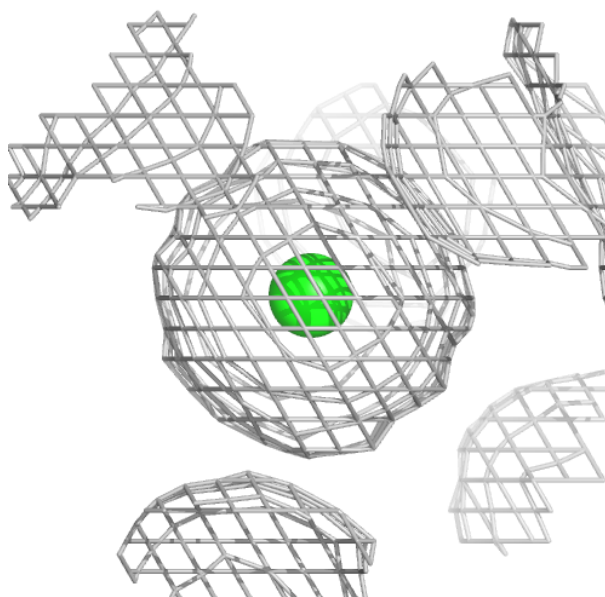
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

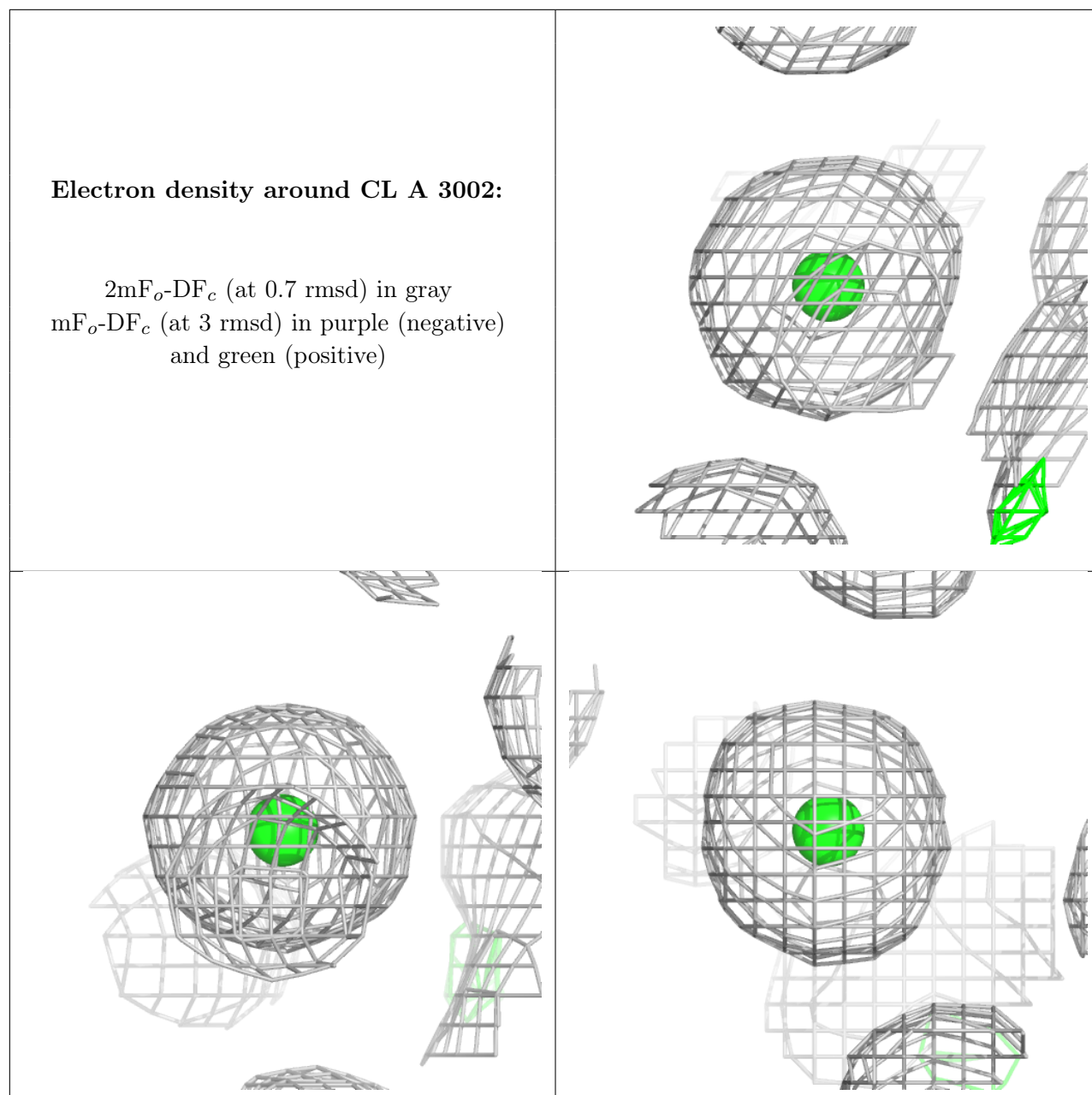




Electron density around CL D 3001:

$2mF_o-DF_c$ (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.