Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2023 – 06:25 pm GMT

PDB ID	:	8BPN
Title	:	The structure of thiocyanate dehydrogenase mutant form with Phe 436 replaced by Gln from Thioalkalivibrio paradoxus
Authors	:	Varfolomeeva, L.A.; Solovieva, A.Y.; Shipkov, N.S.; Kulikova, O.G.; Dergousova, N.I.; Rakitina, T.V.; Boyko, K.M.; Tikhonova, T.V.; Popov, V.O.
Deposited on	:	2023-01-09
Resolution	:	1.99 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:

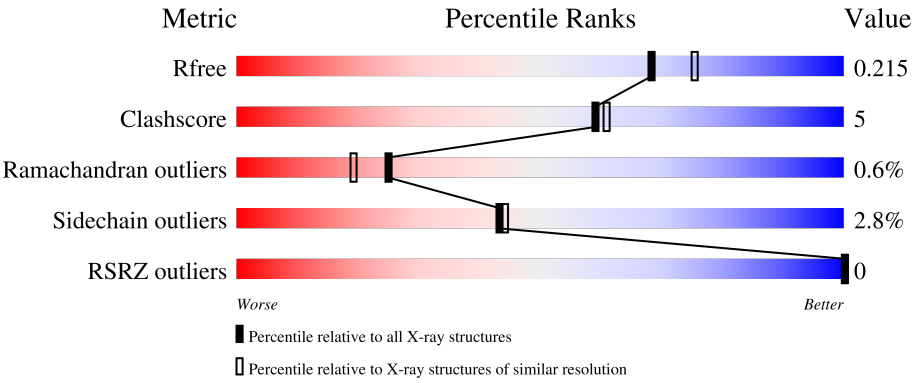
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	494	83% 12% 5%
1	B	494	82% 12% • 5%
1	C	494	79% 15% • 5%
1	D	494	81% 12% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14967 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 Twin-arginine translocation signal domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	1	0
			3631	2317	606	689	19			
1	B	467	Total	C	N	O	S	0	0	0
			3631	2317	606	690	18			
1	C	467	Total	C	N	O	S	0	0	0
			3627	2314	606	689	18			
1	D	467	Total	C	N	O	S	0	1	0
			3632	2318	606	690	18			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	MET	-	initiating methionine	UNP W0DP94
A	56	SER	-	expression tag	UNP W0DP94
A	57	TYR	-	expression tag	UNP W0DP94
A	58	TYR	-	expression tag	UNP W0DP94
A	59	HIS	-	expression tag	UNP W0DP94
A	60	HIS	-	expression tag	UNP W0DP94
A	61	HIS	-	expression tag	UNP W0DP94
A	62	HIS	-	expression tag	UNP W0DP94
A	63	HIS	-	expression tag	UNP W0DP94
A	64	HIS	-	expression tag	UNP W0DP94
A	65	ASP	-	expression tag	UNP W0DP94
A	66	TYR	-	expression tag	UNP W0DP94
A	67	ASP	-	expression tag	UNP W0DP94
A	68	ILE	-	expression tag	UNP W0DP94
A	69	PRO	-	expression tag	UNP W0DP94
A	70	THR	-	expression tag	UNP W0DP94
A	71	THR	-	expression tag	UNP W0DP94
A	72	GLU	-	expression tag	UNP W0DP94
A	73	ASN	-	expression tag	UNP W0DP94
A	74	LEU	-	expression tag	UNP W0DP94
A	75	TYR	-	expression tag	UNP W0DP94

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Chain	Residue	Modelled	Actual	Comment	Reference
A	76	PHE	-	expression tag	UNP W0DP94
A	77	GLN	-	expression tag	UNP W0DP94
A	78	GLY	-	expression tag	UNP W0DP94
A	79	ALA	-	expression tag	UNP W0DP94
A	80	MET	-	expression tag	UNP W0DP94
A	81	GLY	-	expression tag	UNP W0DP94
A	436	GLN	PHE	engineered mutation	UNP W0DP94
B	55	MET	-	initiating methionine	UNP W0DP94
B	56	SER	-	expression tag	UNP W0DP94
B	57	TYR	-	expression tag	UNP W0DP94
B	58	TYR	-	expression tag	UNP W0DP94
B	59	HIS	-	expression tag	UNP W0DP94
B	60	HIS	-	expression tag	UNP W0DP94
B	61	HIS	-	expression tag	UNP W0DP94
B	62	HIS	-	expression tag	UNP W0DP94
B	63	HIS	-	expression tag	UNP W0DP94
B	64	HIS	-	expression tag	UNP W0DP94
B	65	ASP	-	expression tag	UNP W0DP94
B	66	TYR	-	expression tag	UNP W0DP94
B	67	ASP	-	expression tag	UNP W0DP94
B	68	ILE	-	expression tag	UNP W0DP94
B	69	PRO	-	expression tag	UNP W0DP94
B	70	THR	-	expression tag	UNP W0DP94
B	71	THR	-	expression tag	UNP W0DP94
B	72	GLU	-	expression tag	UNP W0DP94
B	73	ASN	-	expression tag	UNP W0DP94
B	74	LEU	-	expression tag	UNP W0DP94
B	75	TYR	-	expression tag	UNP W0DP94
B	76	PHE	-	expression tag	UNP W0DP94
B	77	GLN	-	expression tag	UNP W0DP94
B	78	GLY	-	expression tag	UNP W0DP94
B	79	ALA	-	expression tag	UNP W0DP94
B	80	MET	-	expression tag	UNP W0DP94
B	81	GLY	-	expression tag	UNP W0DP94
B	436	GLN	PHE	engineered mutation	UNP W0DP94
C	55	MET	-	initiating methionine	UNP W0DP94
C	56	SER	-	expression tag	UNP W0DP94
C	57	TYR	-	expression tag	UNP W0DP94
C	58	TYR	-	expression tag	UNP W0DP94
C	59	HIS	-	expression tag	UNP W0DP94
C	60	HIS	-	expression tag	UNP W0DP94
C	61	HIS	-	expression tag	UNP W0DP94

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Chain	Residue	Modelled	Actual	Comment	Reference
C	62	HIS	-	expression tag	UNP W0DP94
C	63	HIS	-	expression tag	UNP W0DP94
C	64	HIS	-	expression tag	UNP W0DP94
C	65	ASP	-	expression tag	UNP W0DP94
C	66	TYR	-	expression tag	UNP W0DP94
C	67	ASP	-	expression tag	UNP W0DP94
C	68	ILE	-	expression tag	UNP W0DP94
C	69	PRO	-	expression tag	UNP W0DP94
C	70	THR	-	expression tag	UNP W0DP94
C	71	THR	-	expression tag	UNP W0DP94
C	72	GLU	-	expression tag	UNP W0DP94
C	73	ASN	-	expression tag	UNP W0DP94
C	74	LEU	-	expression tag	UNP W0DP94
C	75	TYR	-	expression tag	UNP W0DP94
C	76	PHE	-	expression tag	UNP W0DP94
C	77	GLN	-	expression tag	UNP W0DP94
C	78	GLY	-	expression tag	UNP W0DP94
C	79	ALA	-	expression tag	UNP W0DP94
C	80	MET	-	expression tag	UNP W0DP94
C	81	GLY	-	expression tag	UNP W0DP94
C	436	GLN	PHE	engineered mutation	UNP W0DP94
D	55	MET	-	initiating methionine	UNP W0DP94
D	56	SER	-	expression tag	UNP W0DP94
D	57	TYR	-	expression tag	UNP W0DP94
D	58	TYR	-	expression tag	UNP W0DP94
D	59	HIS	-	expression tag	UNP W0DP94
D	60	HIS	-	expression tag	UNP W0DP94
D	61	HIS	-	expression tag	UNP W0DP94
D	62	HIS	-	expression tag	UNP W0DP94
D	63	HIS	-	expression tag	UNP W0DP94
D	64	HIS	-	expression tag	UNP W0DP94
D	65	ASP	-	expression tag	UNP W0DP94
D	66	TYR	-	expression tag	UNP W0DP94
D	67	ASP	-	expression tag	UNP W0DP94
D	68	ILE	-	expression tag	UNP W0DP94
D	69	PRO	-	expression tag	UNP W0DP94
D	70	THR	-	expression tag	UNP W0DP94
D	71	THR	-	expression tag	UNP W0DP94
D	72	GLU	-	expression tag	UNP W0DP94
D	73	ASN	-	expression tag	UNP W0DP94
D	74	LEU	-	expression tag	UNP W0DP94
D	75	TYR	-	expression tag	UNP W0DP94

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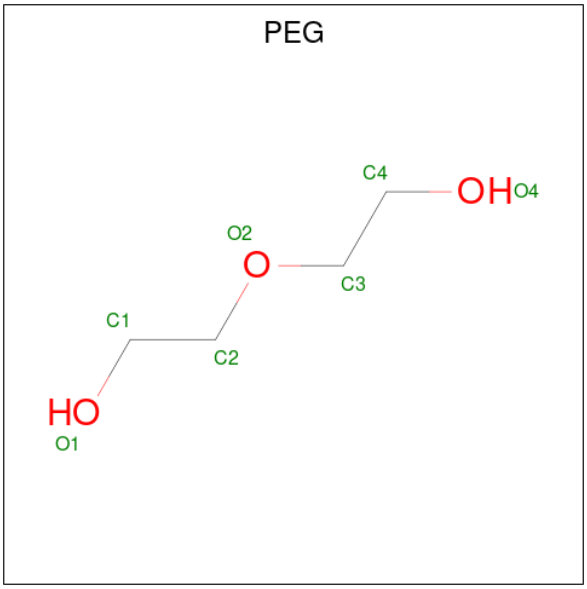
Chain	Residue	Modelled	Actual	Comment	Reference
D	76	PHE	-	expression tag	UNP W0DP94
D	77	GLN	-	expression tag	UNP W0DP94
D	78	GLY	-	expression tag	UNP W0DP94
D	79	ALA	-	expression tag	UNP W0DP94
D	80	MET	-	expression tag	UNP W0DP94
D	81	GLY	-	expression tag	UNP W0DP94
D	436	GLN	PHE	engineered mutation	UNP W0DP94

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cu 2 2	0	0
3	B	2	Total Cu 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	2	Total Cu 2 2	0	0
3	D	2	Total Cu 2 2	0	0

- Molecule 4 is water.

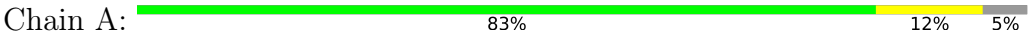
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	96	Total O 96 96	0	0
4	B	123	Total O 123 123	0	0
4	C	86	Total O 86 86	0	0
4	D	119	Total O 119 119	0	0

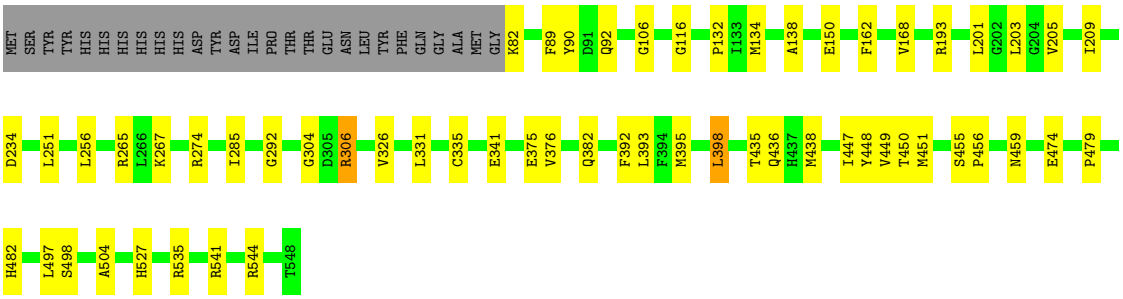
3 Residue-property plots (i)

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: Twin-arginine translocation signal domain-containing protein

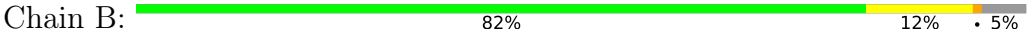
Chain A:

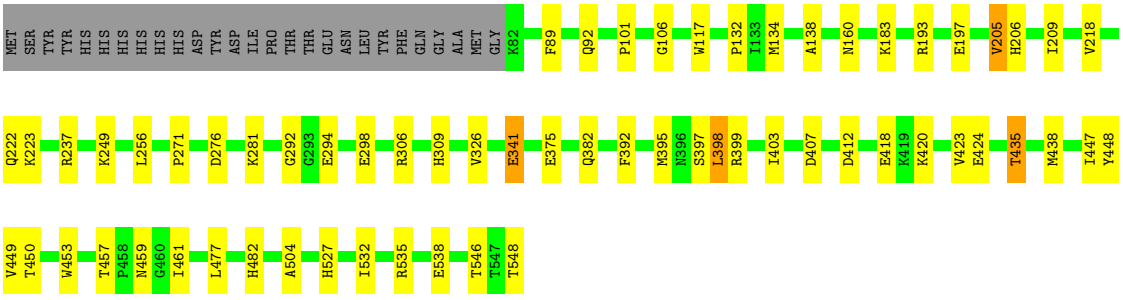




• Molecule 1: Twin-arginine translocation signal domain-containing protein

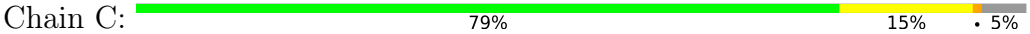
Chain B:

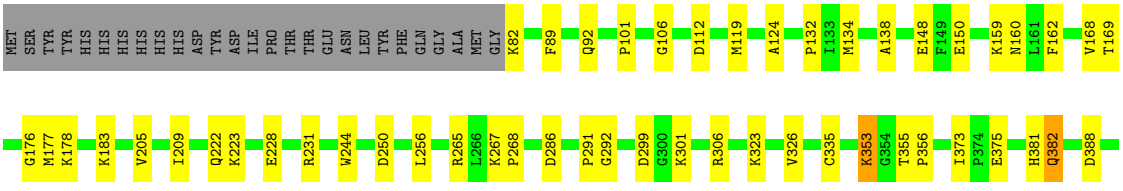


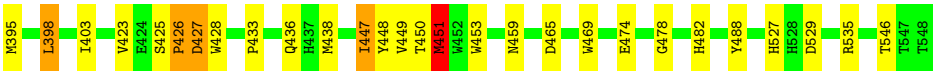


• Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain C:

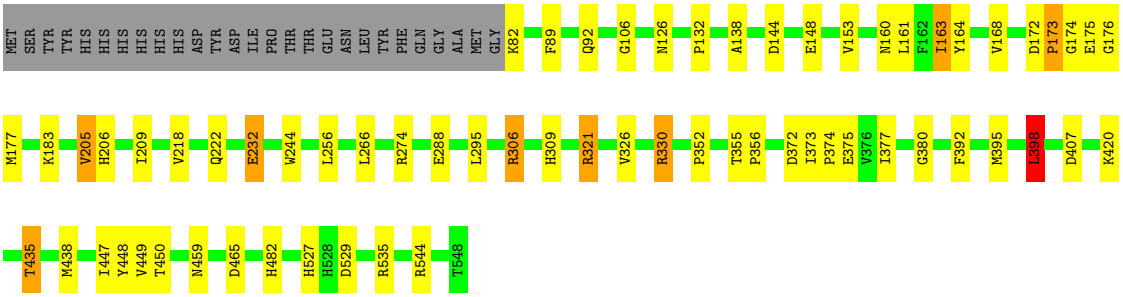






• Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.56Å 162.12Å 90.86Å 90.00° 119.80° 90.00°	Depositor
Resolution (Å)	81.06 – 1.99 81.06 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.7 (81.06-1.99) 92.7 (81.06-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.174 , 0.214 0.174 , 0.215	Depositor DCC
R_{free} test set	6911 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	21.3	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 23.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.035 for -h-l,k,h 0.035 for l,k,-h-l 0.039 for h,-k,-h-l 0.039 for -h-l,-k,l 0.437 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14967	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, 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	0.80	3/3737 (0.1%)	1.17	13/5100 (0.3%)
1	B	0.83	5/3733 (0.1%)	1.22	15/5095 (0.3%)
1	C	0.78	2/3729 (0.1%)	1.17	17/5090 (0.3%)
1	D	0.80	2/3738 (0.1%)	1.20	14/5101 (0.3%)
All	All	0.80	12/14937 (0.1%)	1.19	59/20386 (0.3%)

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	B	0	2
1	C	0	1
All	All	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	341	GLU	CD-OE2	7.82	1.34	1.25
1	A	498	SER	CA-CB	-7.32	1.42	1.52
1	B	197	GLU	CD-OE2	7.14	1.33	1.25
1	C	228	GLU	CD-OE1	-7.10	1.17	1.25
1	C	150	GLU	CD-OE1	-6.94	1.18	1.25
1	B	538	GLU	CD-OE1	6.33	1.32	1.25
1	B	418	GLU	CD-OE2	5.61	1.31	1.25
1	D	288	GLU	CD-OE1	-5.23	1.19	1.25
1	A	234	ASP	CG-OD2	-5.20	1.13	1.25
1	D	175	GLU	CD-OE2	5.18	1.31	1.25
1	B	298	GLU	CD-OE1	5.06	1.31	1.25
1	B	397	SER	CB-OG	5.04	1.48	1.42

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	306	ARG	CG-CD-NE	-15.50	79.25	111.80
1	B	306	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	B	306	ARG	CD-NE-CZ	9.83	137.37	123.60
1	B	101	PRO	N-CD-CG	-9.62	88.77	103.20
1	C	306	ARG	CG-CD-NE	-9.52	91.80	111.80
1	C	134	MET	CG-SD-CE	-9.45	85.09	100.20
1	B	535	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	B	134	MET	CG-SD-CE	-8.91	85.94	100.20
1	D	232	GLU	CB-CG-CD	8.75	137.83	114.20
1	A	306	ARG	CG-CD-NE	-8.60	93.74	111.80
1	D	535	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	B	306	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	D	535	ARG	CD-NE-CZ	8.01	134.81	123.60
1	D	274	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	A	544	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	B	412	ASP	CB-CA-C	7.59	125.58	110.40
1	A	535	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	C	388	ASP	CB-CG-OD1	7.50	125.05	118.30
1	C	388	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	C	231	ARG	NE-CZ-NH1	-7.26	116.67	120.30
1	C	535	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	A	274	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	535	ARG	CD-NE-CZ	7.06	133.49	123.60
1	A	134	MET	CG-SD-CE	-6.98	89.03	100.20
1	D	330	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	A	193	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	C	488	TYR	CB-CG-CD1	-6.72	116.97	121.00
1	D	535	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	D	465	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	C	101	PRO	N-CD-CG	-6.30	93.74	103.20
1	C	427	ASP	N-CA-CB	-6.30	99.27	110.60
1	C	535	ARG	CD-NE-CZ	6.21	132.29	123.60
1	A	479	PRO	CB-CA-C	-6.08	96.79	112.00
1	D	172	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	A	193	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	D	544	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	B	504	ALA	CB-CA-C	5.91	118.97	110.10
1	D	153	VAL	CA-CB-CG1	5.88	119.72	110.90
1	B	535	ARG	CG-CD-NE	-5.78	99.66	111.80
1	C	451	MET	CG-SD-CE	-5.68	91.11	100.20
1	B	399	ARG	CG-CD-NE	-5.48	100.30	111.80
1	C	231	ARG	NE-CZ-NH2	5.46	123.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	237	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	193	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	D	535	ARG	CG-CD-NE	-5.32	100.62	111.80
1	A	306	ARG	CD-NE-CZ	5.26	130.97	123.60
1	A	541	ARG	CG-CD-NE	-5.26	100.76	111.80
1	D	321	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	A	306	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	B	535	ARG	CD-NE-CZ	5.14	130.80	123.60
1	C	426	PRO	C-N-CA	5.14	134.54	121.70
1	B	546	THR	CA-CB-OG1	-5.12	98.24	109.00
1	D	144	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	C	223	LYS	CB-CA-C	-5.11	100.19	110.40
1	C	546	THR	CA-CB-OG1	-5.04	98.41	109.00
1	A	306	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	C	353	LYS	CB-CA-C	5.04	120.47	110.40
1	D	274	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	C	178	LYS	CD-CE-NZ	-5.01	100.17	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	309	HIS	Sidechain
1	B	435	THR	Peptide
1	C	169	THR	Mainchain

5.2 Too-close contacts (i)

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	3631	0	3504	27	0
1	B	3631	0	3502	33	0
1	C	3627	0	3499	37	0
1	D	3632	0	3506	39	0
2	A	7	0	10	0	0
2	B	7	0	10	2	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	96	0	0	1	0
4	B	123	0	0	2	0
4	C	86	0	0	0	0
4	D	119	0	0	3	0
All	All	14967	0	14031	134	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 (134) 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:C:148:GLU:OE1	1:C:183:LYS:HE3	1.53	1.08
1:C:382:GLN:HE21	1:C:436:GLN:HA	1.14	1.06
1:C:382:GLN:NE2	1:C:436:GLN:HA	1.75	1.01
1:B:292:GLY:HA2	1:B:398:LEU:HD21	1.49	0.93
1:B:292:GLY:HA2	1:B:398:LEU:CD2	2.00	0.91
1:D:148:GLU:OE2	1:D:183[A]:LYS:HE2	1.70	0.91
1:A:292:GLY:HA2	1:A:398:LEU:HD22	1.59	0.84
1:C:292:GLY:HA2	1:C:398:LEU:HD22	1.62	0.82
1:B:461:ILE:HD12	1:B:477:LEU:HD11	1.63	0.80
1:D:352:PRO:HB2	1:D:377:ILE:HD12	1.66	0.77
1:C:382:GLN:HE21	1:C:436:GLN:CA	1.97	0.75
1:B:183:LYS:HE3	4:B:712:HOH:O	1.85	0.74
1:C:382:GLN:NE2	1:C:436:GLN:CA	2.50	0.73
1:B:424:GLU:HB3	4:B:805:HOH:O	1.89	0.73
1:D:161:LEU:HD23	1:D:173:PRO:HG3	1.69	0.72
1:A:292:GLY:HA2	1:A:398:LEU:CD2	2.20	0.71
1:B:382:GLN:HE21	1:B:438:MET:HE3	1.56	0.70
1:B:382:GLN:HE21	1:B:438:MET:CE	2.04	0.70
1:C:299:ASP:HB3	1:C:301:LYS:HE3	1.74	0.70
1:A:382:GLN:HG3	1:A:436:GLN:C	2.13	0.68
1:A:265:ARG:HD2	1:A:267:LYS:HE3	1.76	0.67
1:C:292:GLY:HA2	1:C:398:LEU:CD2	2.23	0.67
1:B:382:GLN:HE22	1:B:548:THR:H	1.44	0.66
1:A:435:THR:HG22	1:A:451[A]:MET:HE1	1.77	0.66
1:B:450:THR:HG21	1:B:482:HIS:O	1.96	0.66
1:D:148:GLU:OE2	4:D:701:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451[B]:MET:SD	1:A:474:GLU:OE2	2.57	0.63
1:D:355:THR:HG23	1:D:377:ILE:HD11	1.80	0.62
1:B:89:PHE:O	1:B:92:GLN:HG2	2.00	0.62
1:D:355:THR:HG23	1:D:377:ILE:CD1	2.30	0.62
1:D:160:ASN:HD21	1:D:222:GLN:NE2	1.97	0.61
1:C:450:THR:HG21	1:C:482:HIS:O	2.00	0.61
1:B:292:GLY:HA2	1:B:398:LEU:HD22	1.82	0.60
1:C:89:PHE:O	1:C:92:GLN:HG2	2.02	0.60
1:D:435:THR:CG2	1:D:449:VAL:HG23	2.31	0.60
1:A:450:THR:HG21	1:A:482:HIS:O	2.02	0.59
1:D:148:GLU:OE1	1:D:183[B]:LYS:HE3	2.00	0.59
1:D:435:THR:HG21	1:D:449:VAL:CG2	2.33	0.59
1:D:450:THR:HG21	1:D:482:HIS:O	2.03	0.58
1:C:160:ASN:HD21	1:C:222:GLN:HE22	1.51	0.58
1:D:435:THR:HG21	1:D:449:VAL:HG21	1.85	0.58
1:D:126:ASN:ND2	4:D:709:HOH:O	2.38	0.57
1:A:89:PHE:O	1:A:92:GLN:HG2	2.04	0.57
1:D:435:THR:CG2	1:D:449:VAL:CG2	2.84	0.56
1:B:382:GLN:HG3	1:B:438:MET:HE2	1.88	0.56
1:D:89:PHE:O	1:D:92:GLN:HG2	2.06	0.56
1:C:176:GLY:O	1:C:177:MET:HB2	2.07	0.55
1:C:160:ASN:HD21	1:C:222:GLN:NE2	2.04	0.55
1:C:265:ARG:HD2	1:C:267:LYS:HE3	1.88	0.55
1:A:504:ALA:HB1	1:B:117:TRP:CE3	2.42	0.55
1:C:267:LYS:HB3	1:C:268:PRO:HD2	1.88	0.55
1:B:160:ASN:HD21	1:B:222:GLN:NE2	2.05	0.54
1:C:148:GLU:OE1	1:C:183:LYS:CE	2.43	0.53
1:B:160:ASN:HD21	1:B:222:GLN:HE22	1.54	0.53
1:C:428:TRP:CZ2	1:C:451:MET:HE3	2.44	0.53
1:D:161:LEU:HG	1:D:168:VAL:HG21	1.90	0.53
1:C:159:LYS:HD2	1:C:286:ASP:HB3	1.92	0.52
1:B:294:GLU:HG2	1:B:398:LEU:HD23	1.92	0.51
1:D:435:THR:HG23	1:D:449:VAL:HG23	1.91	0.51
1:D:306:ARG:NH1	1:D:309:HIS:CD2	2.79	0.50
1:D:435:THR:HG23	1:D:450:THR:O	2.12	0.50
1:A:150:GLU:OE2	4:A:701:HOH:O	2.19	0.49
1:C:355:THR:HB	1:C:356:PRO:HD2	1.95	0.49
1:C:459:ASN:HB2	1:C:478:GLY:O	2.12	0.49
1:A:285:ILE:HA	1:A:304:GLY:HA3	1.95	0.49
1:A:162:PHE:CD1	1:A:168:VAL:CG2	2.96	0.48
1:B:403:ILE:HB	1:B:423:VAL:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ILE:HB	1:C:423:VAL:HB	1.94	0.48
1:D:206:HIS:O	1:D:218:VAL:HA	2.14	0.48
1:B:341:GLU:H	1:B:341:GLU:CD	2.17	0.48
1:D:256:LEU:O	1:D:375:GLU:HB2	2.13	0.47
1:D:161:LEU:HD23	1:D:173:PRO:CG	2.42	0.47
1:C:138:ALA:HB1	1:C:209:ILE:HG12	1.97	0.47
1:A:201:LEU:HD21	1:A:203:LEU:HD11	1.95	0.47
1:B:256:LEU:O	1:B:375:GLU:HB2	2.16	0.46
1:C:438:MET:HA	1:C:448:TYR:O	2.15	0.46
1:D:295:LEU:HD11	1:D:398:LEU:HD21	1.97	0.46
1:D:148:GLU:OE1	1:D:183[B]:LYS:CE	2.64	0.46
1:D:106:GLY:HA2	1:D:132:PRO:O	2.16	0.46
1:A:138:ALA:HB1	1:A:209:ILE:HG12	1.97	0.46
1:B:453:TRP:CD2	1:B:457:THR:HG21	2.51	0.46
1:C:256:LEU:O	1:C:375:GLU:HB2	2.16	0.45
1:D:321:ARG:NH1	4:D:710:HOH:O	2.47	0.45
1:C:106:GLY:HA2	1:C:132:PRO:O	2.16	0.45
1:D:138:ALA:HB1	1:D:209:ILE:HG12	1.97	0.45
1:A:326:VAL:CG1	1:A:335:CYS:HB3	2.47	0.45
1:C:326:VAL:CG1	1:C:335:CYS:HB3	2.46	0.45
1:D:407:ASP:HB2	1:D:420:LYS:HD3	1.99	0.45
1:D:326:VAL:HG11	1:D:392:PHE:CZ	2.52	0.45
1:B:435:THR:HA	1:B:450:THR:O	2.17	0.45
1:D:438:MET:HA	1:D:448:TYR:O	2.16	0.45
1:B:117:TRP:CD2	2:B:601:PEG:H41	2.52	0.45
1:A:435:THR:HG22	1:A:451[A]:MET:CE	2.45	0.44
1:B:106:GLY:HA2	1:B:132:PRO:O	2.16	0.44
1:D:163:ILE:HG22	1:D:164:TYR:CE2	2.52	0.44
1:A:106:GLY:HA2	1:A:132:PRO:O	2.18	0.44
1:B:138:ALA:HB1	1:B:209:ILE:HG12	1.99	0.43
1:A:256:LEU:O	1:A:375:GLU:HB2	2.18	0.43
1:A:438:MET:HA	1:A:448:TYR:O	2.18	0.43
1:B:326:VAL:HG11	1:B:392:PHE:CZ	2.52	0.43
1:A:162:PHE:HD1	1:A:168:VAL:CG2	2.31	0.43
1:A:497:LEU:HD13	1:B:117:TRP:CH2	2.53	0.43
1:B:206:HIS:O	1:B:218:VAL:HA	2.18	0.43
1:B:276:ASP:OD1	1:B:281:LYS:HE2	2.18	0.43
1:C:176:GLY:O	1:C:177:MET:CB	2.66	0.43
1:B:407:ASP:HB2	1:B:420:LYS:HD3	2.01	0.43
1:C:124:ALA:HB3	1:C:132:PRO:CB	2.49	0.43
1:D:435:THR:HA	1:D:450:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:GLY:O	1:D:177:MET:HB2	2.19	0.42
1:A:392:PHE:C	1:A:393:LEU:HD12	2.40	0.42
1:C:112:ASP:HB2	1:C:119:MET:SD	2.60	0.42
1:C:168:VAL:H	1:C:168:VAL:HG22	1.55	0.42
1:B:117:TRP:CE2	2:B:601:PEG:H41	2.54	0.42
1:B:205:VAL:HG12	1:B:206:HIS:N	2.34	0.42
1:D:244:TRP:HZ3	1:D:373:ILE:HD12	1.84	0.42
1:A:326:VAL:HG11	1:A:392:PHE:CZ	2.54	0.42
1:A:455:SER:HA	1:A:456:PRO:HA	1.86	0.42
1:C:428:TRP:CE2	1:C:451:MET:HE1	2.55	0.42
1:A:331:LEU:O	1:A:376:VAL:HG11	2.20	0.42
1:B:382:GLN:HE21	1:B:438:MET:HE2	1.79	0.42
1:A:251:LEU:HD23	1:A:251:LEU:HA	1.94	0.41
1:C:427:ASP:OD2	1:C:474:GLU:OE2	2.38	0.41
1:C:433:PRO:HB3	1:C:453:TRP:NE1	2.35	0.41
1:D:148:GLU:OE1	1:D:183[B]:LYS:NZ	2.51	0.41
1:C:428:TRP:CZ2	1:C:451:MET:CE	3.04	0.41
1:D:205:VAL:HG12	1:D:206:HIS:N	2.36	0.41
1:D:355:THR:HB	1:D:356:PRO:HD2	2.02	0.41
1:D:330:ARG:HA	1:D:380:GLY:O	2.21	0.41
1:C:162:PHE:HD1	1:C:168:VAL:CG2	2.34	0.41
1:C:447:ILE:HD11	1:C:469:TRP:HZ3	1.86	0.41
1:B:438:MET:HA	1:B:448:TYR:O	2.21	0.41
1:A:90:TYR:CZ	1:A:116:GLY:HA3	2.56	0.40
1:C:244:TRP:HZ3	1:C:373:ILE:HD12	1.86	0.40
1:D:373:ILE:HA	1:D:374:PRO:HD3	1.93	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	466/494 (94%)	443 (95%)	21 (4%)	2 (0%)	34	30
1	B	465/494 (94%)	438 (94%)	24 (5%)	3 (1%)	25	19
1	C	465/494 (94%)	437 (94%)	24 (5%)	4 (1%)	17	11
1	D	466/494 (94%)	438 (94%)	25 (5%)	3 (1%)	25	19
All	All	1862/1976 (94%)	1756 (94%)	94 (5%)	12 (1%)	25	19

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	LEU
1	B	398	LEU
1	C	398	LEU
1	D	174	GLY
1	D	398	LEU
1	B	205	VAL
1	B	249	LYS
1	C	205	VAL
1	C	323	LYS
1	D	205	VAL
1	A	205	VAL
1	C	381	HIS

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	390/416 (94%)	383 (98%)	7 (2%)	59	63
1	B	389/416 (94%)	380 (98%)	9 (2%)	50	53
1	C	389/416 (94%)	375 (96%)	14 (4%)	35	34
1	D	390/416 (94%)	376 (96%)	14 (4%)	35	34
All	All	1558/1664 (94%)	1514 (97%)	44 (3%)	43	44

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LYS
1	A	306	ARG
1	A	395	MET
1	A	447	ILE
1	A	449	VAL
1	A	459	ASN
1	A	527	HIS
1	B	223	LYS
1	B	271	PRO
1	B	341	GLU
1	B	395	MET
1	B	447	ILE
1	B	449	VAL
1	B	459	ASN
1	B	527	HIS
1	B	532	ILE
1	C	82	LYS
1	C	250	ASP
1	C	291	PRO
1	C	353	LYS
1	C	382	GLN
1	C	395	MET
1	C	425	SER
1	C	426	PRO
1	C	447	ILE
1	C	449	VAL
1	C	451	MET
1	C	465	ASP
1	C	527	HIS
1	C	529	ASP
1	D	82	LYS
1	D	163	ILE
1	D	173	PRO
1	D	232	GLU
1	D	266	LEU
1	D	306	ARG
1	D	372	ASP
1	D	395	MET
1	D	398	LEU
1	D	435	THR
1	D	447	ILE
1	D	459	ASN
1	D	527	HIS

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Mol	Chain	Res	Type
1	D	529	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	382	GLN
1	A	434	ASN
1	B	126	ASN
1	B	222	GLN
1	B	382	GLN
1	C	126	ASN
1	C	222	GLN
1	C	382	GLN
1	D	126	ASN
1	D	222	GLN
1	D	309	HIS
1	D	434	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	PEG	B	601	-	6,6,6	0.33	0	5,5,5	0.32	0
2	PEG	A	601	-	6,6,6	0.42	0	5,5,5	0.34	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	PEG	B	601	-	-	3/4/4/4	-
2	PEG	A	601	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	PEG	O2-C3-C4-O4
2	B	601	PEG	C4-C3-O2-C2
2	B	601	PEG	C1-C2-O2-C3
2	A	601	PEG	C1-C2-O2-C3

There are no ring outliers.

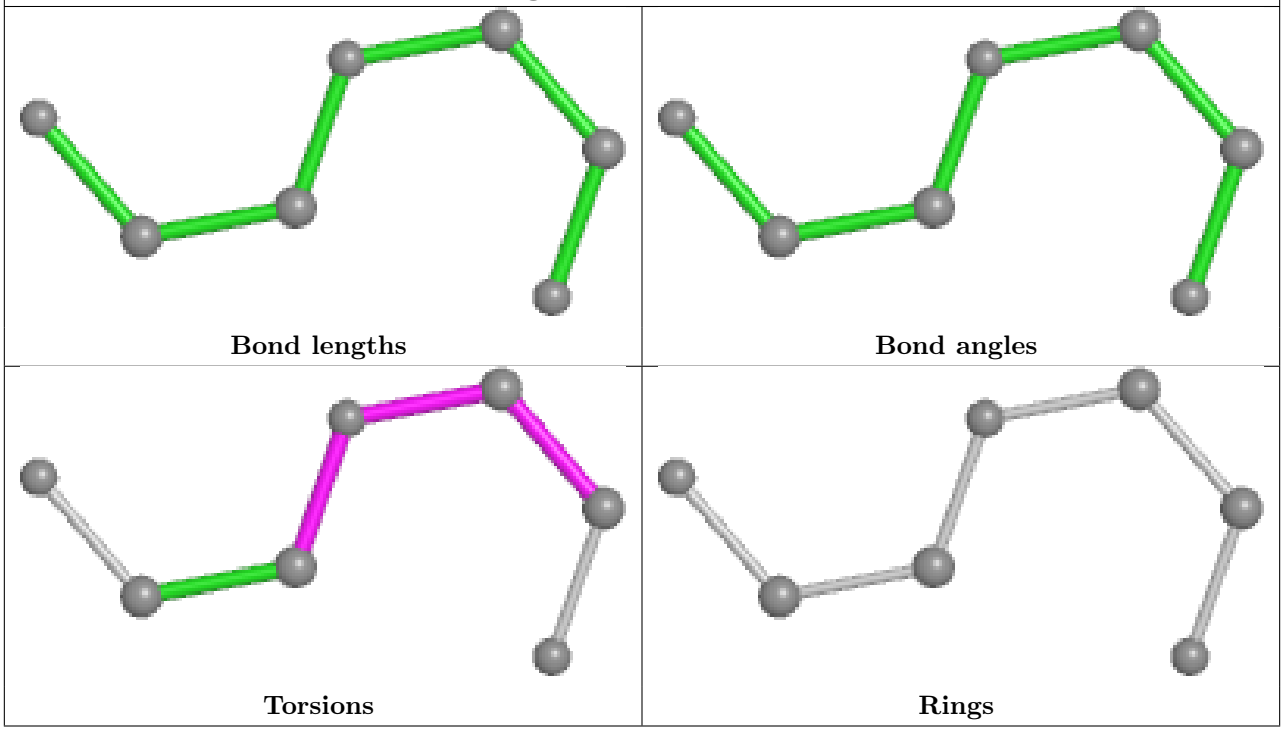
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	PEG	2	0

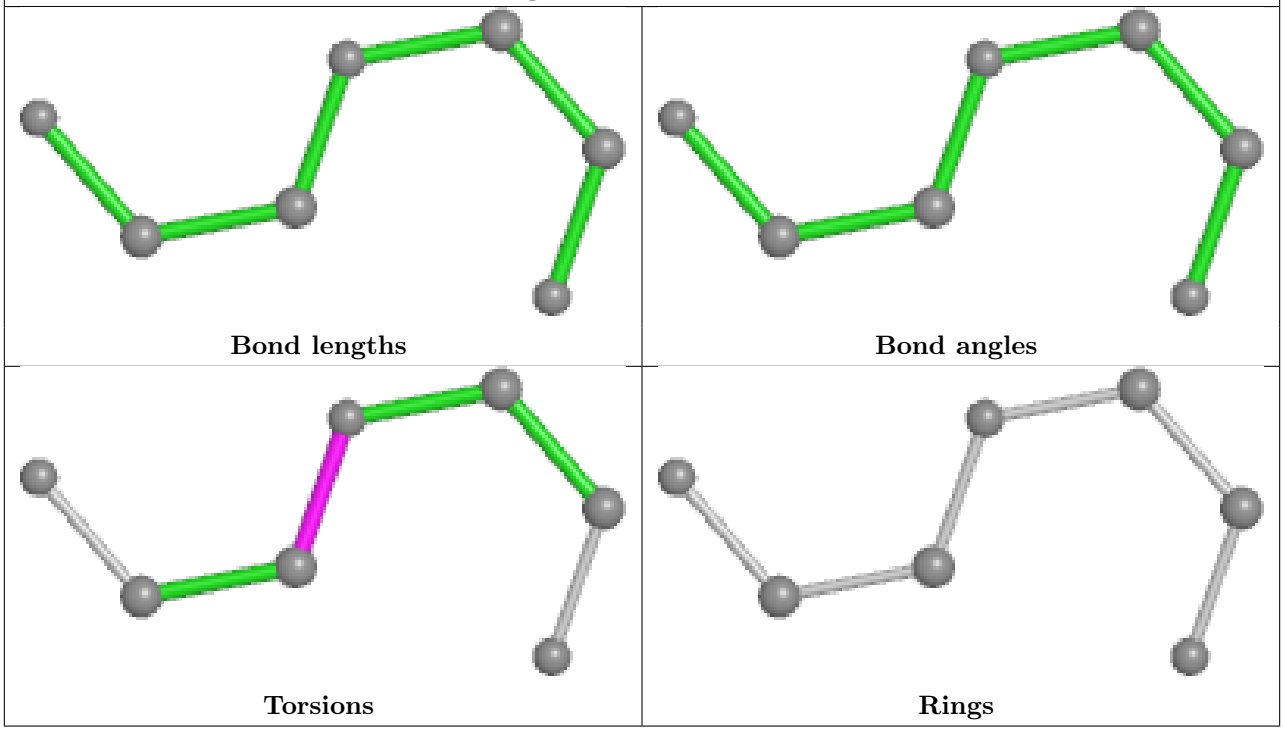
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PEG B 601



Ligand PEG A 601



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^{th} 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	467/494 (94%)	-0.28	0	100	100	11, 22, 36, 59	0
1	B	467/494 (94%)	-0.35	0	100	100	10, 20, 31, 44	0
1	C	467/494 (94%)	-0.30	0	100	100	12, 22, 34, 43	0
1	D	467/494 (94%)	-0.31	0	100	100	12, 21, 32, 51	0
All	All	1868/1976 (94%)	-0.31	0	100	100	10, 21, 34, 59	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PEG	A	601	7/7	0.84	0.20	18,21,26,32	7
2	PEG	B	601	7/7	0.94	0.17	12,15,17,19	7
3	CU	A	603	1/1	0.99	0.10	26,26,26,26	0
3	CU	C	601	1/1	0.99	0.09	25,25,25,25	0

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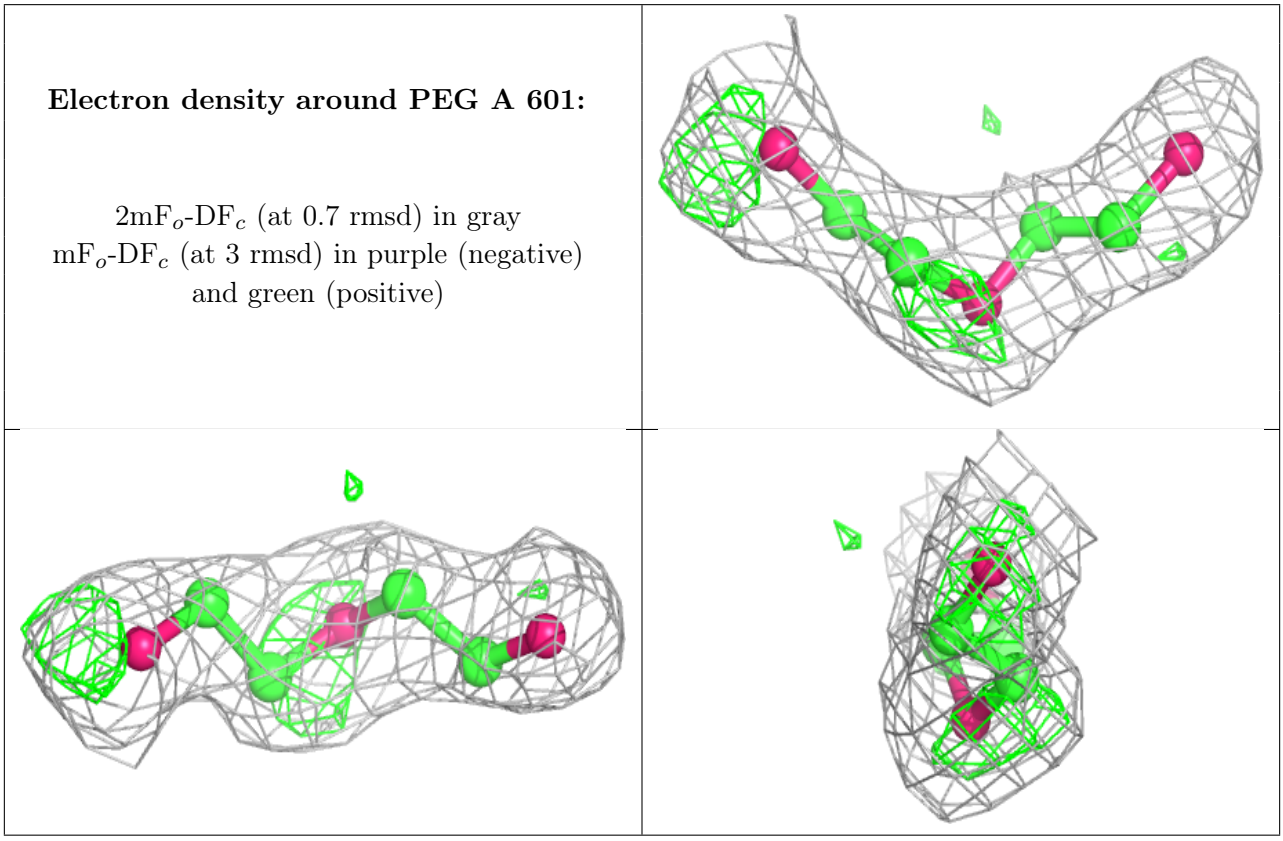
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CU	D	602	1/1	0.99	0.06	25,25,25,25	0
3	CU	B	603	1/1	1.00	0.05	20,20,20,20	0
3	CU	A	602	1/1	1.00	0.06	24,24,24,24	0
3	CU	C	602	1/1	1.00	0.06	22,22,22,22	0
3	CU	D	601	1/1	1.00	0.09	21,21,21,21	0
3	CU	B	602	1/1	1.00	0.04	19,19,19,19	1

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.

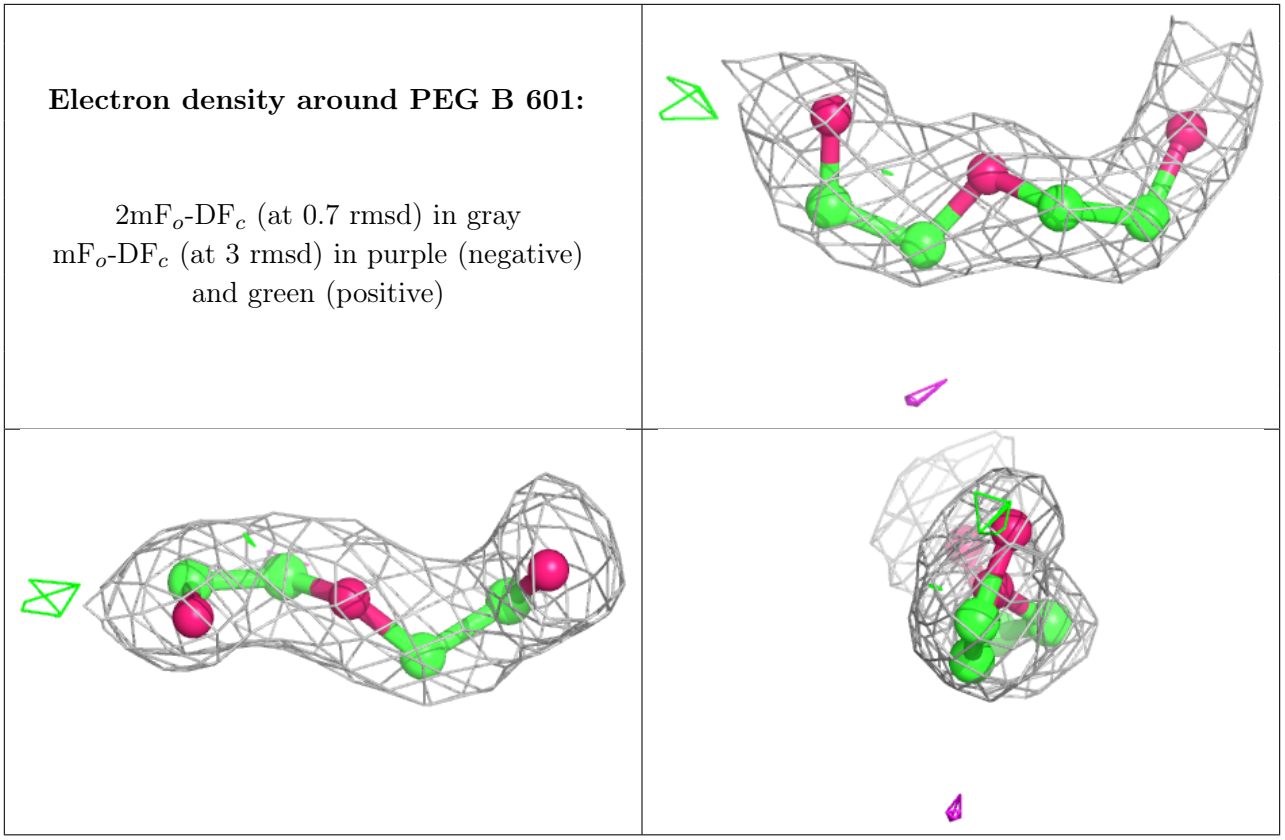
Electron density around PEG A 601:

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



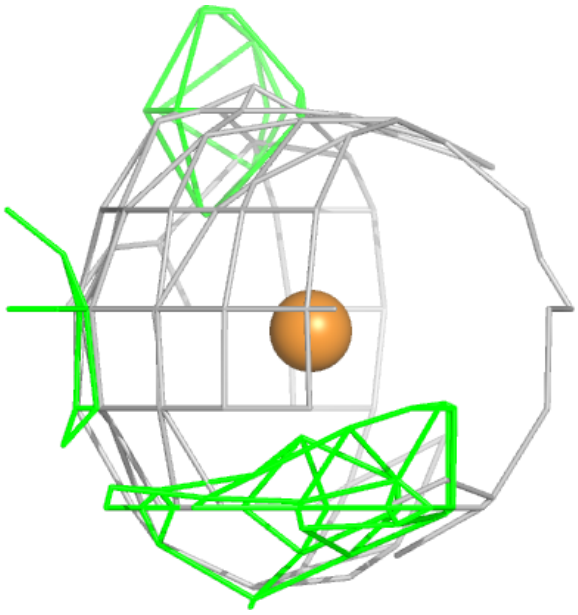
Electron density around PEG B 601:

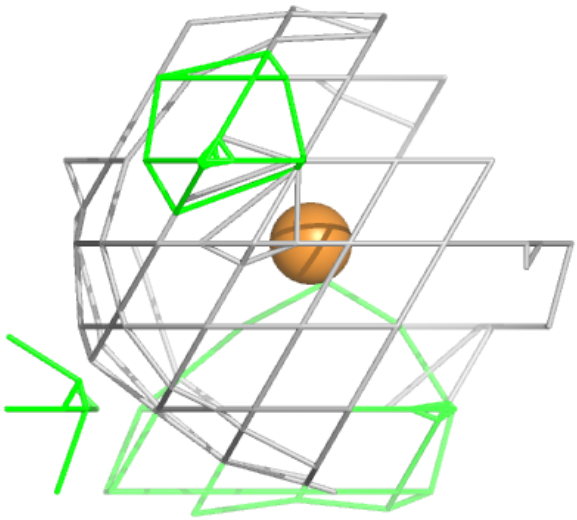
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

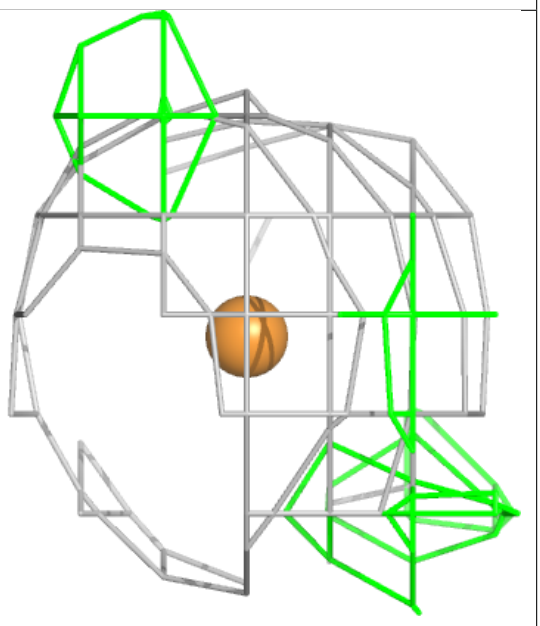


Electron density around CU A 603:

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







Electron density around CU C 601:

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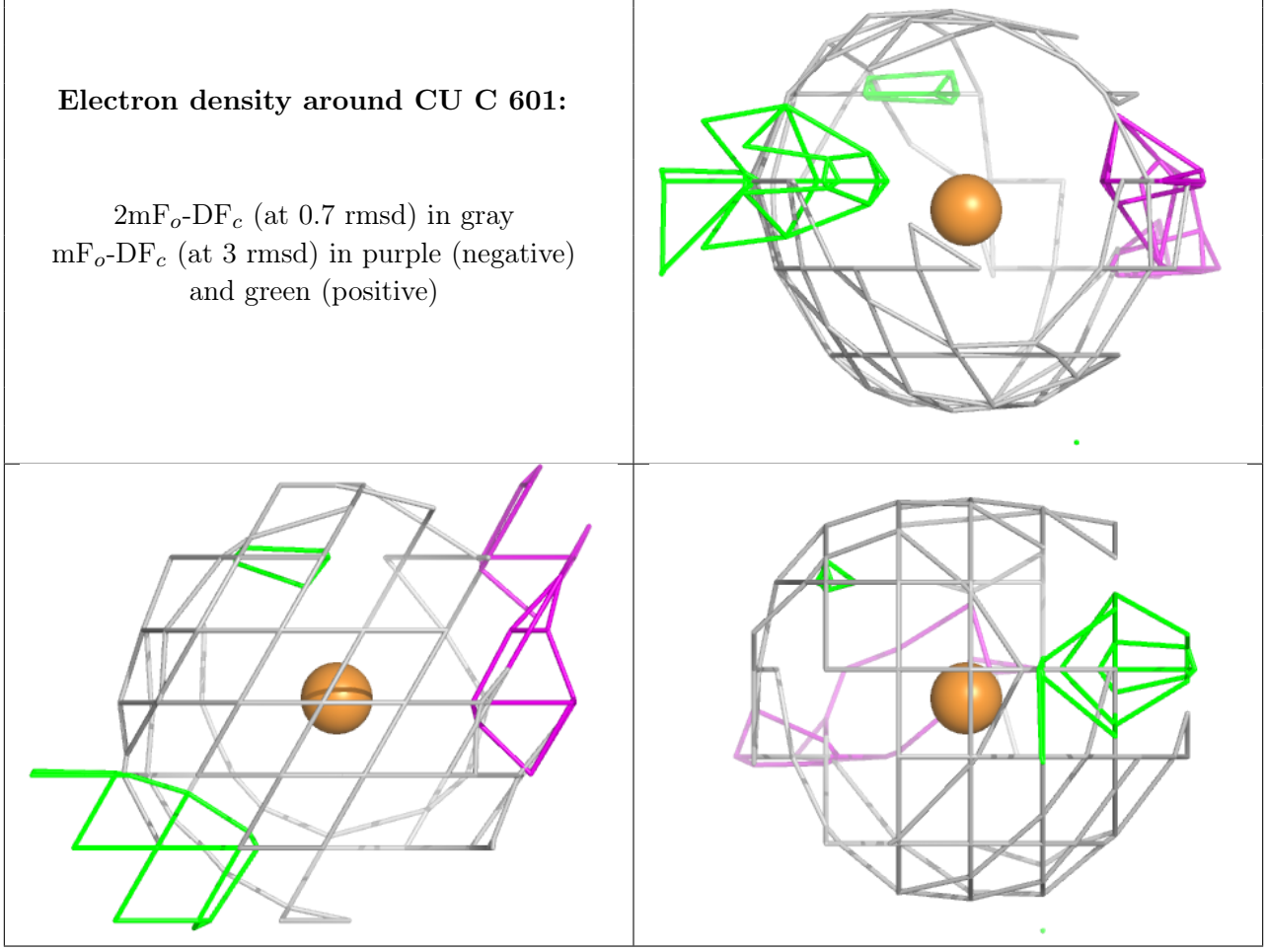
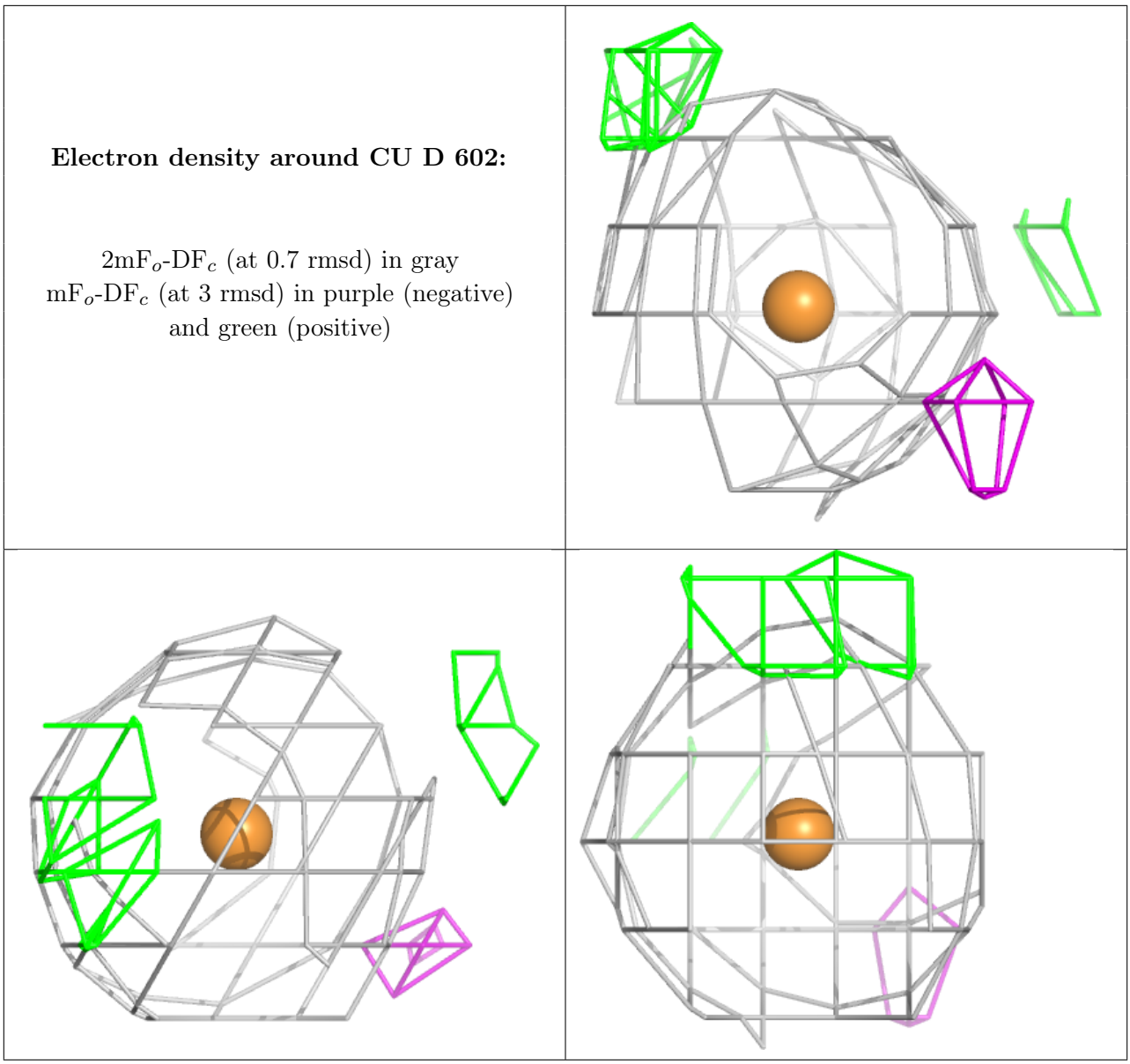
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



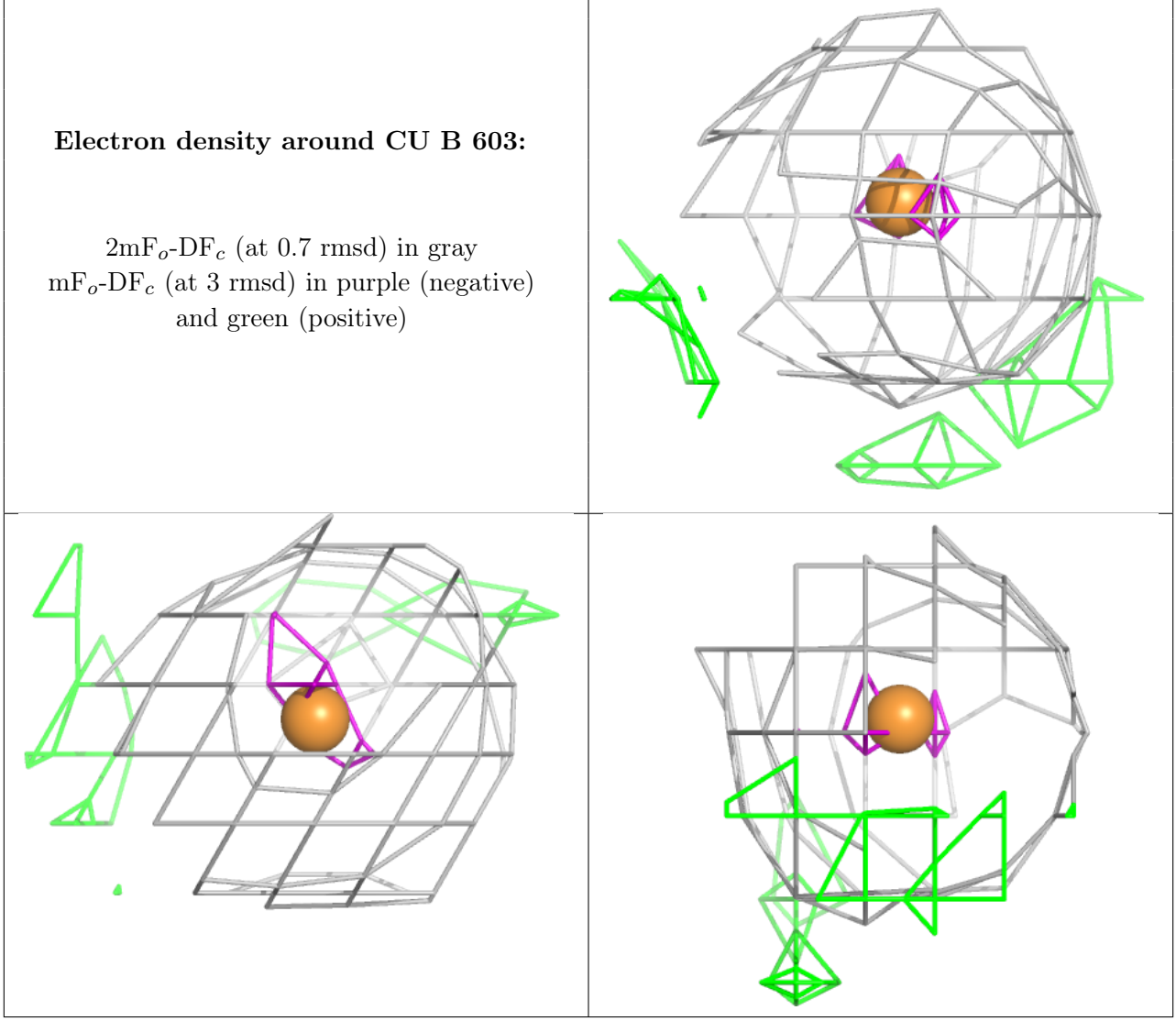
Electron density around CU D 602:

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



Electron density around CU B 603:

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



Electron density around CU A 602:

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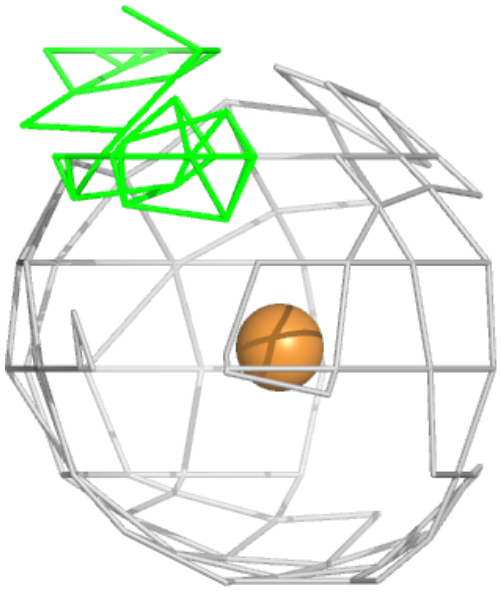
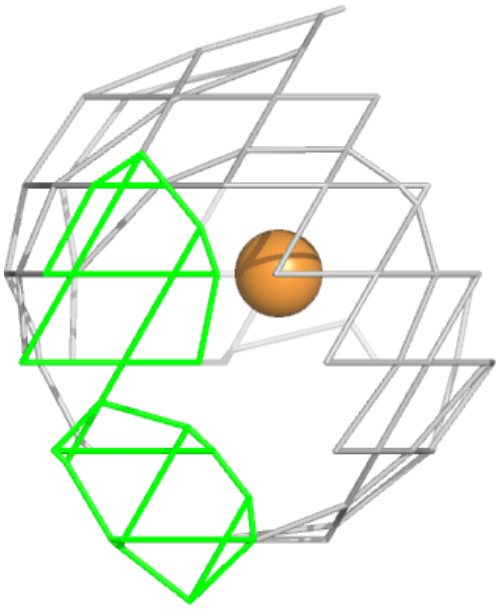
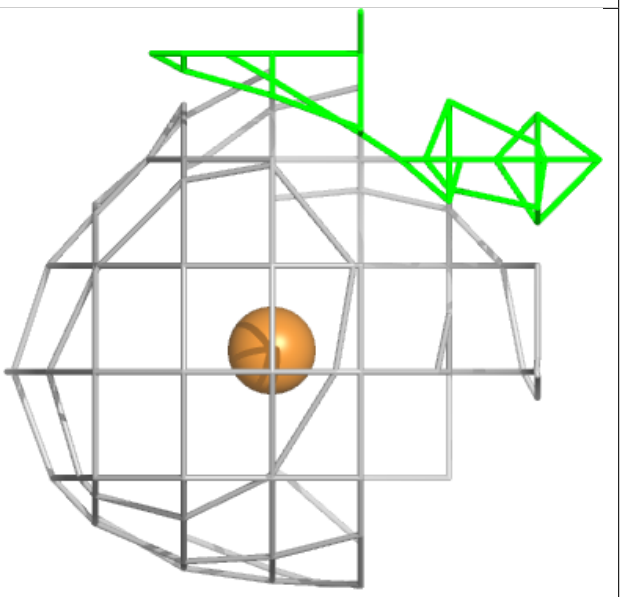
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

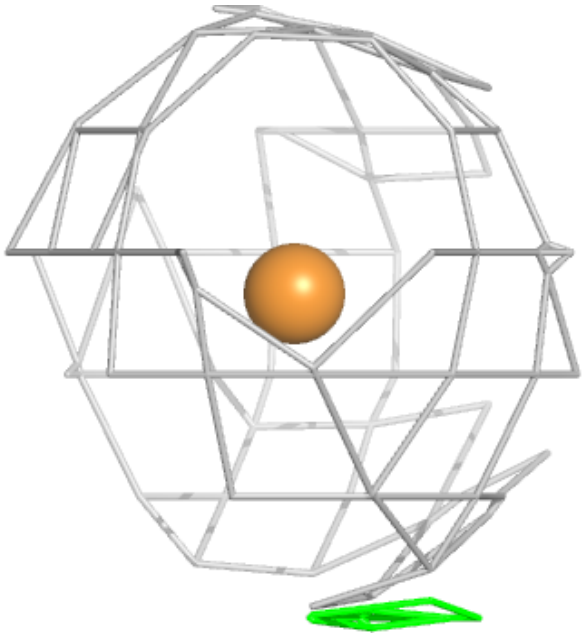


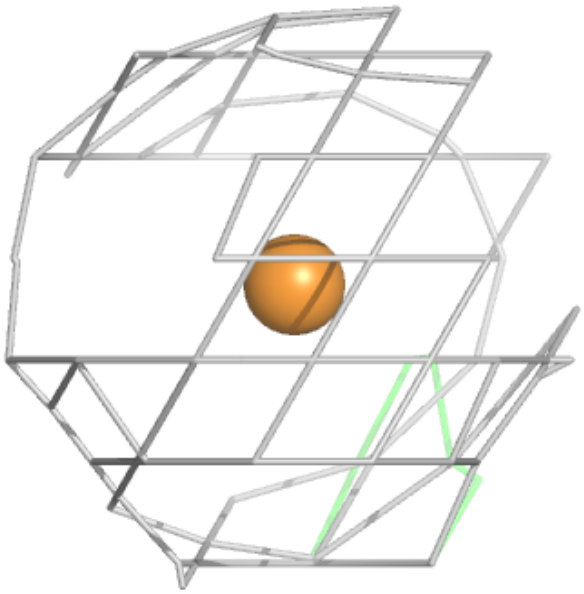


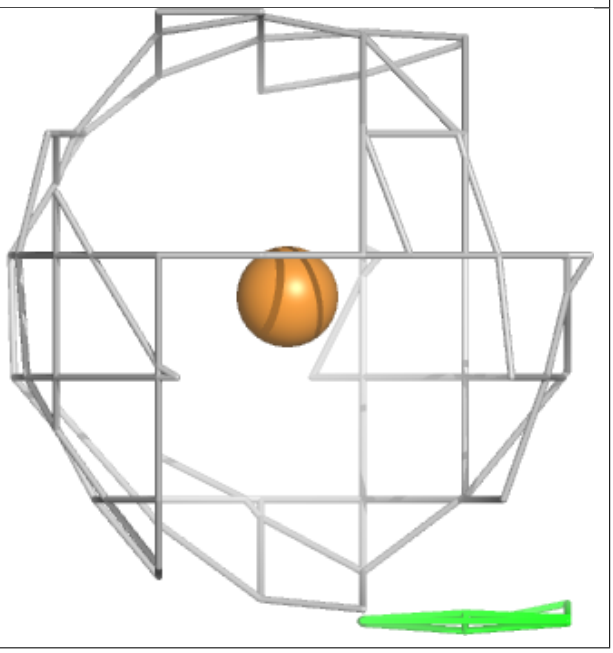


Electron density around CU C 602:

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

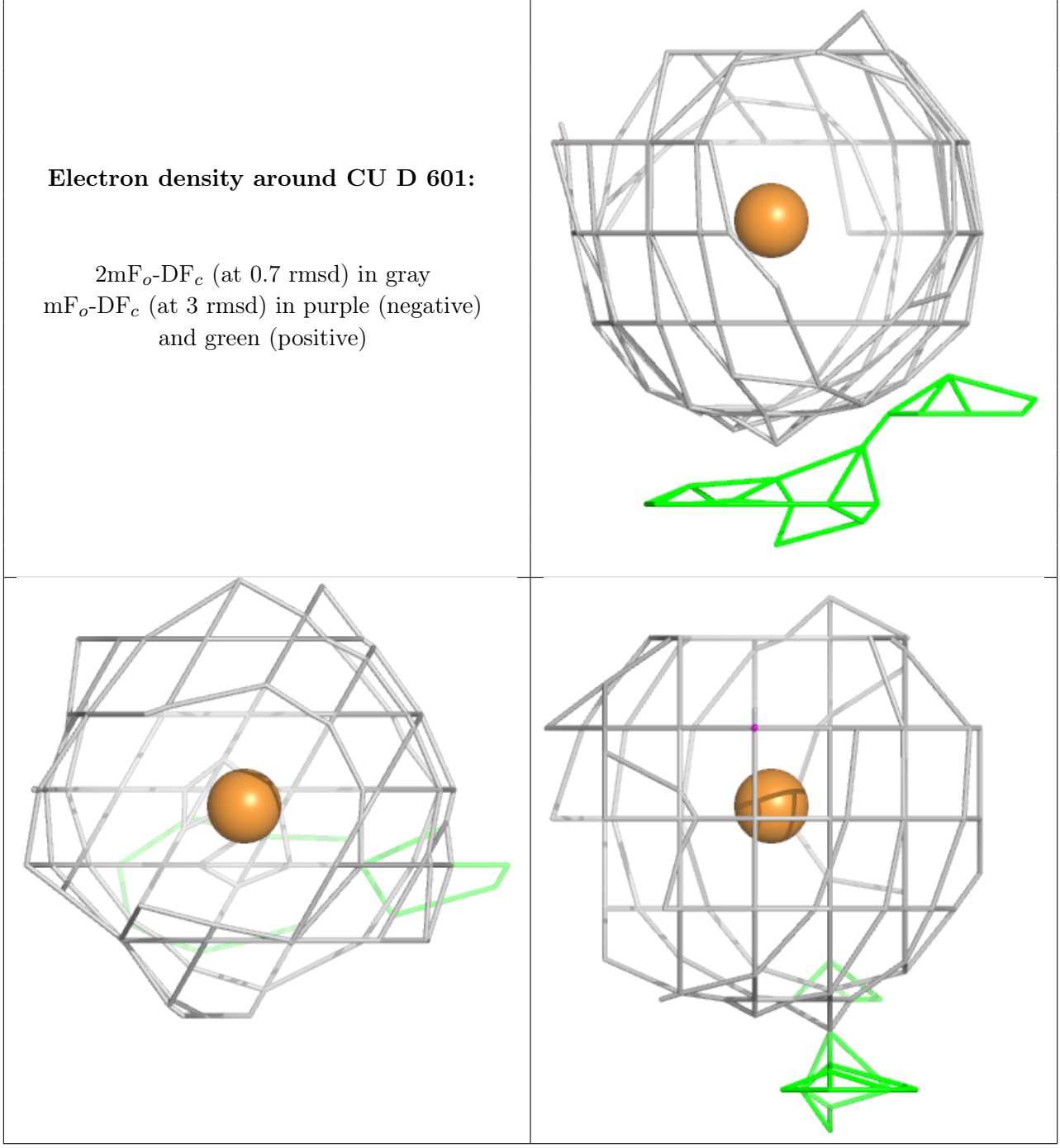






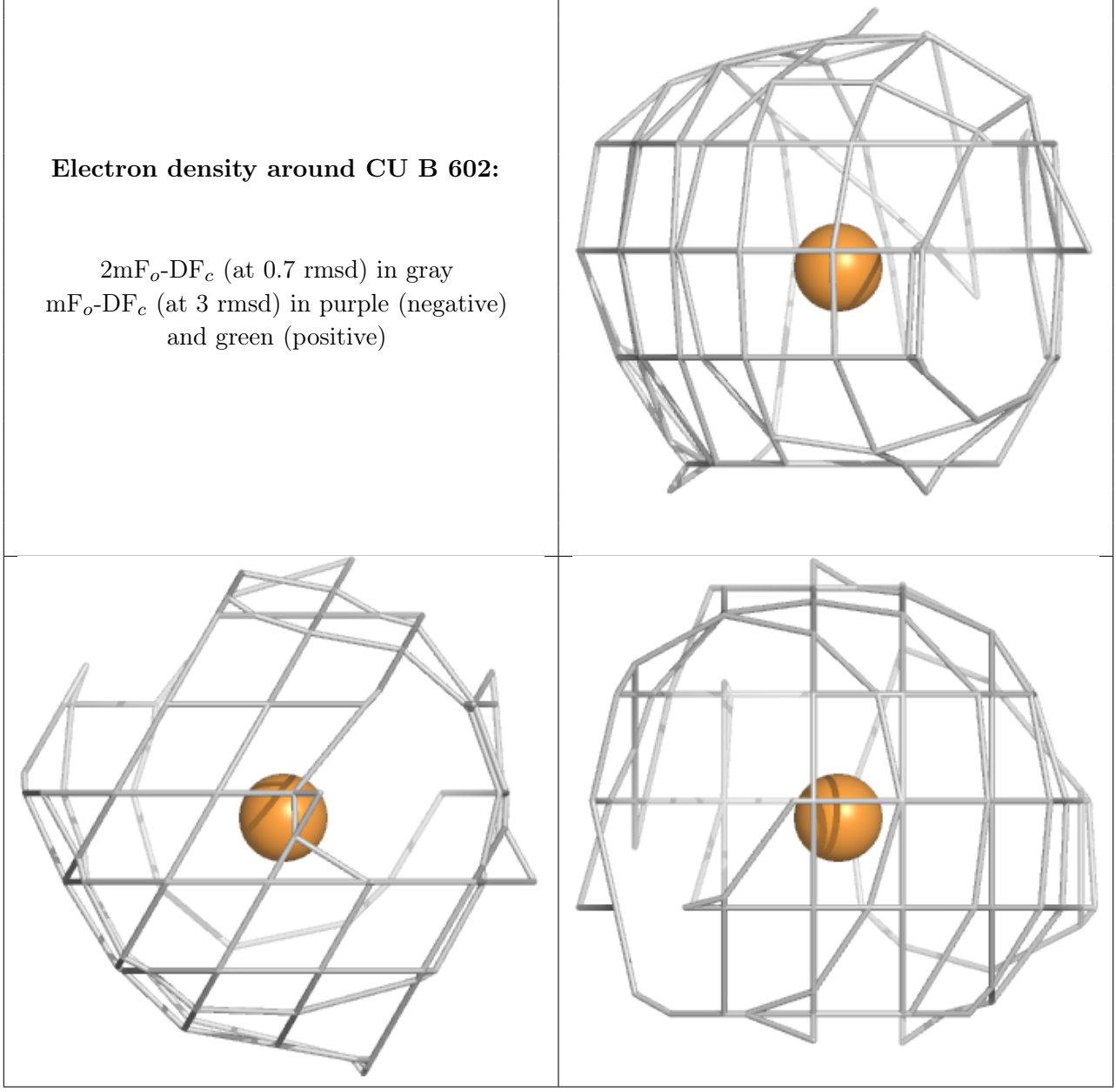
Electron density around CU D 601:

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



Electron density around CU B 602:

$2mF_o$-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.