



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2021 – 04:25 PM GMT

PDB ID : 7AQ6
Title : Pseudomonas stutzeri nitrous oxide reductase mutant, H583F
Authors : Zhang, L.; Bill, E.; Kroneck, P.M.H.; Einsle, O.
Deposited on : 2020-10-20
Resolution : 1.51 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 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 : 2.16
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) : 2.16

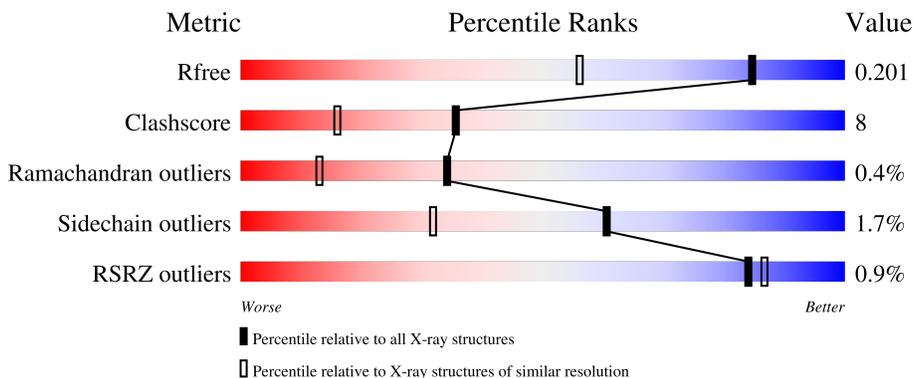
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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	646	
1	B	646	

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	FMT	A	716	-	-	X	-
6	FMT	B	2206	-	-	X	-
6	FMT	B	2211	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 10426 atoms, of which 6 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.

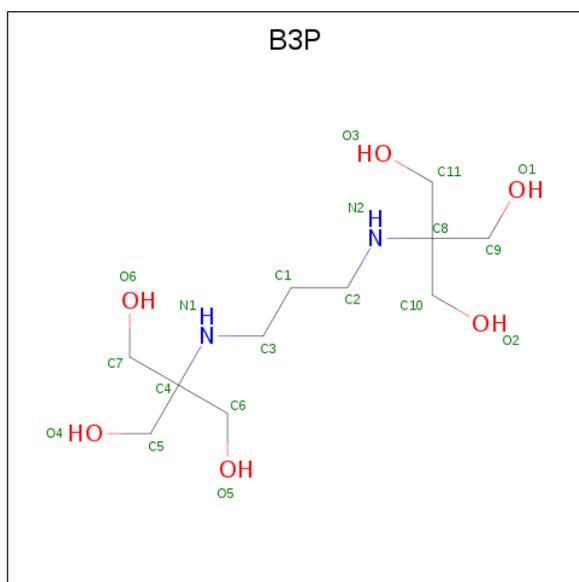
- Molecule 1 is a protein called Nitrous-oxide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	586	4639	2936	794	877	32	0	6	0
1	B	588	4650	2948	797	873	32	0	2	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	583	PHE	HIS	engineered mutation	UNP P19573
A	639	TRP	-	expression tag	UNP P19573
A	640	SER	-	expression tag	UNP P19573
A	641	HIS	-	expression tag	UNP P19573
A	642	PRO	-	expression tag	UNP P19573
A	643	GLN	-	expression tag	UNP P19573
A	644	PHE	-	expression tag	UNP P19573
A	645	GLU	-	expression tag	UNP P19573
A	646	LYS	-	expression tag	UNP P19573
B	583	PHE	HIS	engineered mutation	UNP P19573
B	639	TRP	-	expression tag	UNP P19573
B	640	SER	-	expression tag	UNP P19573
B	641	HIS	-	expression tag	UNP P19573
B	642	PRO	-	expression tag	UNP P19573
B	643	GLN	-	expression tag	UNP P19573
B	644	PHE	-	expression tag	UNP P19573
B	645	GLU	-	expression tag	UNP P19573
B	646	LYS	-	expression tag	UNP P19573

- Molecule 2 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: C₁₁H₂₆N₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
2	A	1	Total	C	N	O	0	0
			19	11	2	6		
2	B	1	Total	C	N	O	0	0
			19	11	2	6		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

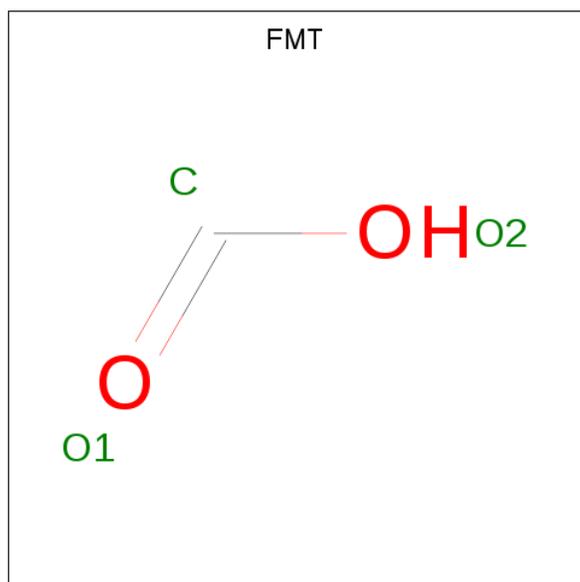
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	K	0	0
			1	1		

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

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 3 1 2	0	0
6	A	1	Total C O 3 1 2	0	0
6	A	1	Total C O 3 1 2	0	0
6	A	1	Total C O 3 1 2	0	0
6	A	1	Total C O 3 1 2	0	0
6	A	1	Total C O 3 1 2	0	0
6	A	1	Total C O 3 1 2	0	0
6	A	1	Total C H O 5 1 2 2	0	0
6	A	1	Total C H O 5 1 2 2	0	0

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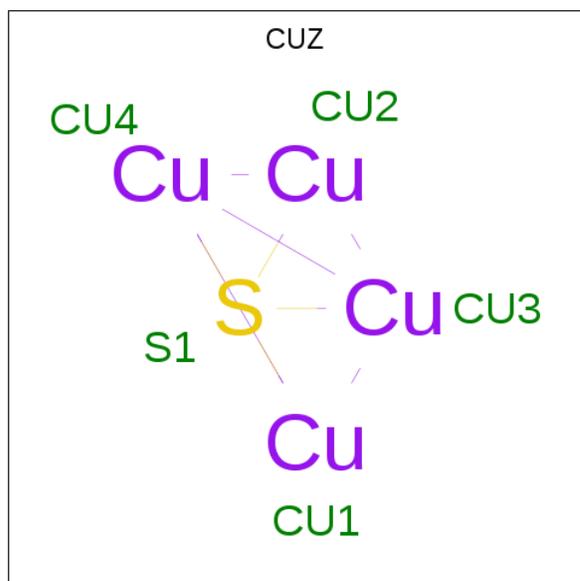
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C H O 5 1 2 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

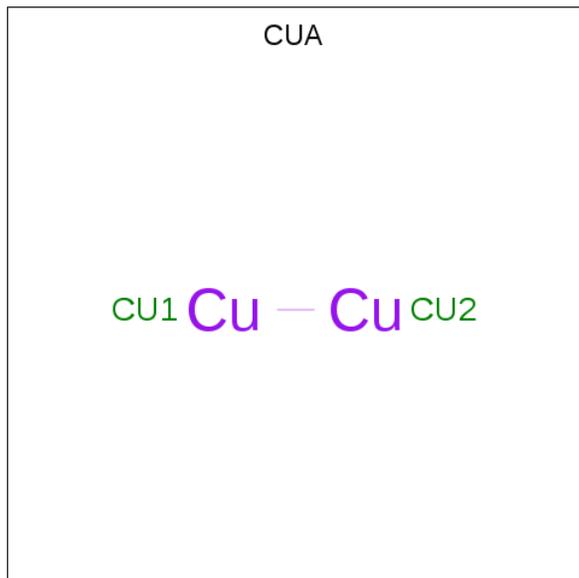
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Cl 1 1	0	0
7	A	1	Total Cl 1 1	0	0

- Molecule 8 is (MU-4-SULFIDO)-TETRA-NUCLEAR COPPER ION (three-letter code: CUZ) (formula: Cu₄S) (labeled as "Ligand of Interest" by depositor).



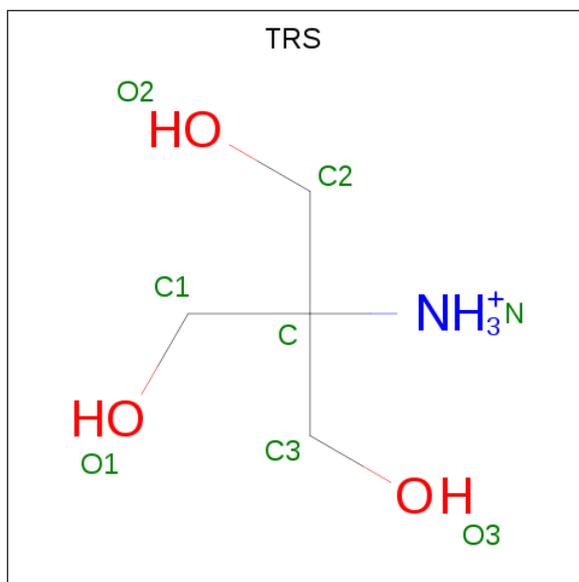
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cu S 5 4 1	0	0
8	B	1	Total Cu S 5 4 1	0	0

- Molecule 9 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Cu 2 2	0	0
9	B	1	Total Cu 2 2	0	0

- Molecule 10 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $\text{C}_4\text{H}_{12}\text{NO}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	558	Total	O	0	0
			558	558		
11	B	463	Total	O	0	0
			463	463		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.05Å 76.59Å 108.63Å 90.00° 93.34° 90.00°	Depositor
Resolution (Å)	108.44 – 1.51 108.44 – 1.51	Depositor EDS
% Data completeness (in resolution range)	64.7 (108.44-1.51) 64.9 (108.44-1.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.51Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.156 , 0.200 0.157 , 0.201	Depositor DCC
R_{free} test set	5773 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10426	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA, K, B3P, CUZ, CUA, TRS, CA, FMT

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	0.50	1/4766 (0.0%)	0.66	3/6451 (0.0%)
1	B	0.46	0/4775	0.63	1/6470 (0.0%)
All	All	0.48	1/9541 (0.0%)	0.64	4/12921 (0.0%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	CYS	CB-SG	-7.63	1.69	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	PRO	C-N-CA	-8.36	100.81	121.70
1	A	303	LEU	CA-CB-CG	-7.75	97.48	115.30
1	A	85	LEU	CA-CB-CG	5.68	128.37	115.30
1	B	580	ASP	CB-CG-OD1	5.64	123.37	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	336	TYR	Peptide

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	4639	0	4521	72	0
1	B	4650	0	4505	88	1
2	A	19	0	26	1	0
2	B	19	0	26	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	30	4	10	4	0
6	B	12	2	4	5	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	5	0	0	0	0
8	B	5	0	0	0	0
9	A	2	0	0	0	0
9	B	2	0	0	0	0
10	A	8	0	12	0	1
11	A	558	0	0	17	5
11	B	463	0	0	20	2
All	All	10420	6	9104	149	7

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 8.

The worst 5 of 149 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:469[A]:GLU:HG3	1:A:492:GLU:HA	1.38	1.03
1:A:543:LYS:NZ	11:A:801:HOH:O	1.91	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ASP:HB2	11:A:1242:HOH:O	1.64	0.96
1:A:577:GLN:HG2	11:A:1098:HOH:O	1.70	0.91
1:A:267:MET:HE2	1:B:628:GLU:HG3	1.52	0.91

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1329:HOH:O	11:A:1356:HOH:O[2_546]	1.80	0.40
11:B:2663:HOH:O	11:B:2711:HOH:O[2_645]	1.87	0.33
11:B:2637:HOH:O	11:B:2683:HOH:O[2_645]	2.09	0.11
11:A:1327:HOH:O	11:A:1329:HOH:O[2_556]	2.11	0.09
10:A:711:TRS:O3	11:A:1354:HOH:O[2_546]	2.16	0.04

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	590/646 (91%)	567 (96%)	21 (4%)	2 (0%)	41 18
1	B	588/646 (91%)	564 (96%)	21 (4%)	3 (0%)	29 9
All	All	1178/1292 (91%)	1131 (96%)	42 (4%)	5 (0%)	34 13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	342	LYS
1	A	342	LYS
1	B	416	GLU
1	A	176	ALA
1	B	176	ALA

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	507/545 (93%)	499 (98%)	8 (2%)	62	35
1	B	505/545 (93%)	496 (98%)	9 (2%)	59	29
All	All	1012/1090 (93%)	995 (98%)	17 (2%)	60	32

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	621	PHE
1	B	78	HIS
1	B	434	LEU
1	A	620	TRP
1	B	483	LEU

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	78	HIS
1	B	494	HIS

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 [i](#)

Of 29 ligands modelled in this entry, 8 are monoatomic - leaving 21 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

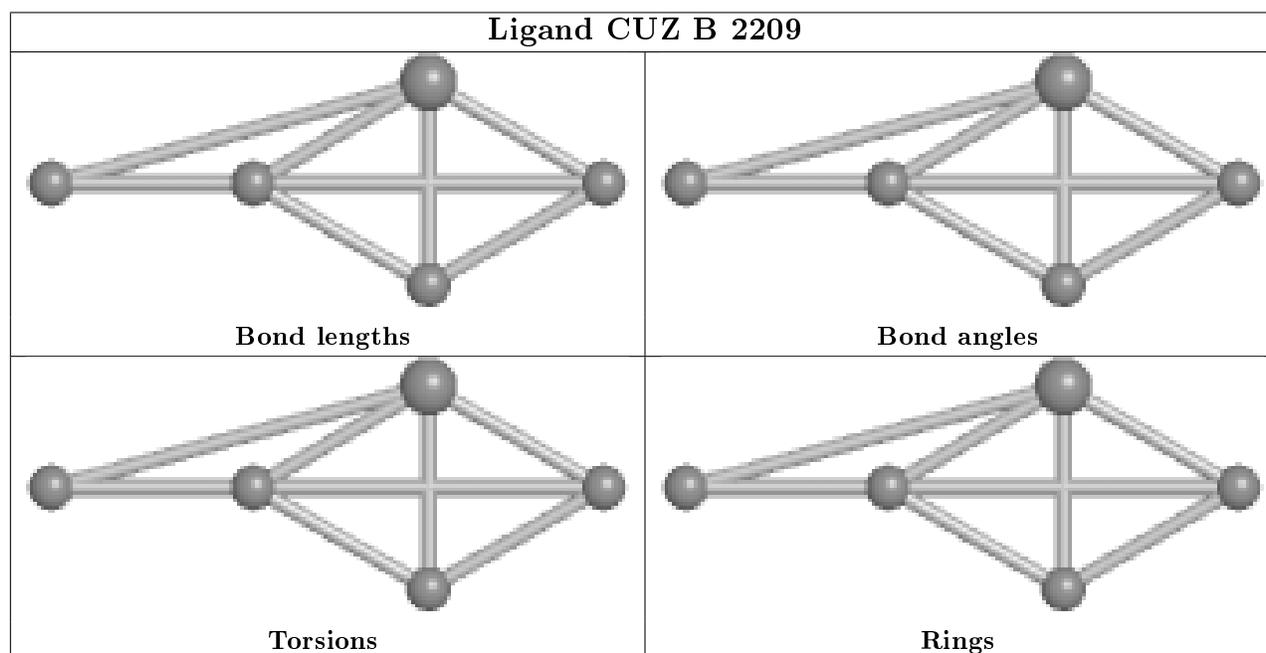
There are no chirality outliers.

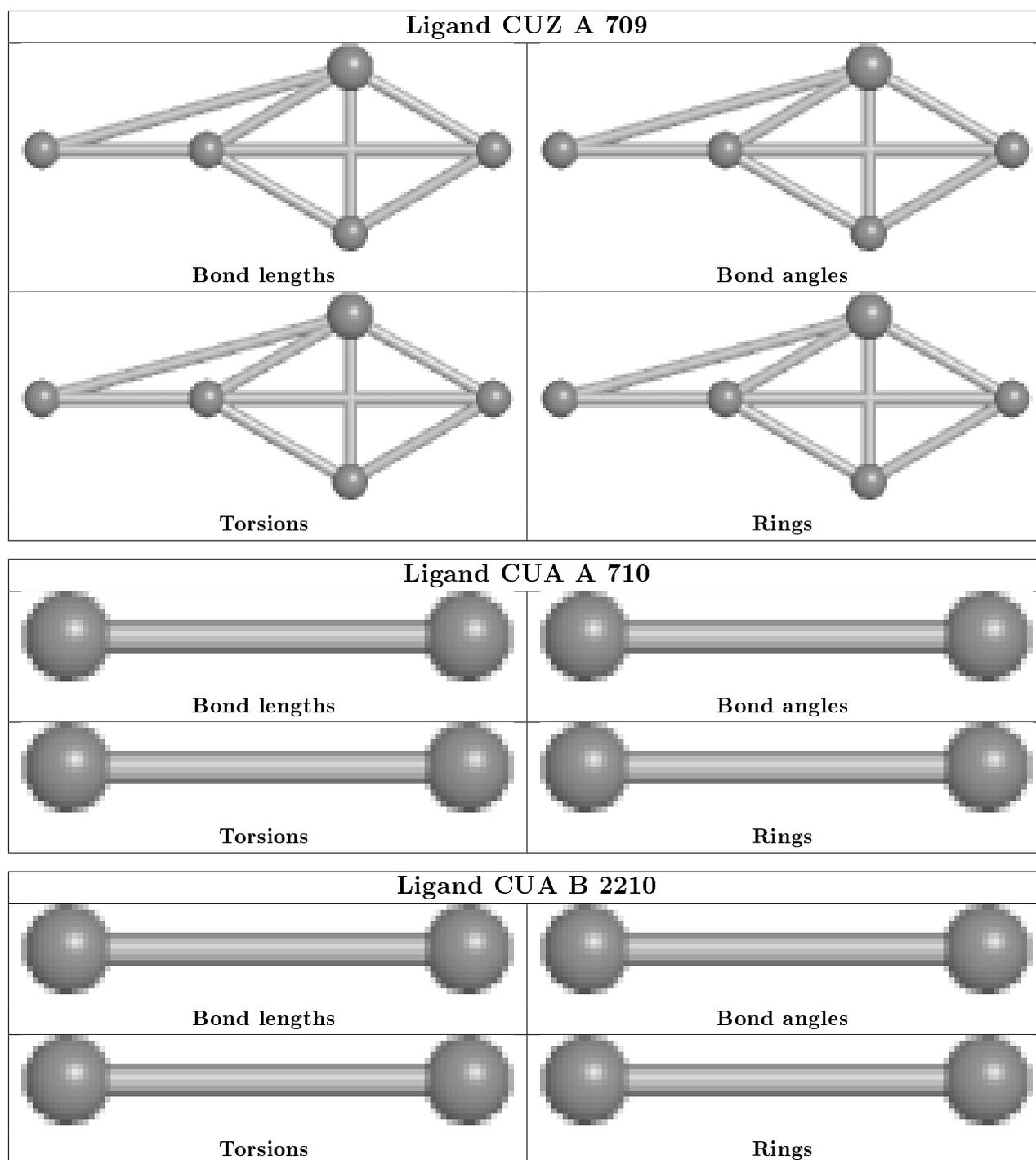
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	586/646 (90%)	-0.57	5 (0%) 84 87	12, 23, 46, 75	0
1	B	588/646 (91%)	-0.49	6 (1%) 82 85	14, 28, 51, 83	0
All	All	1174/1292 (90%)	-0.53	11 (0%) 84 87	12, 26, 48, 83	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	644	PHE	3.4
1	B	643	GLN	3.2
1	B	60	ILE	3.2
1	A	269	ARG	2.9
1	A	262	PHE	2.6

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](#)

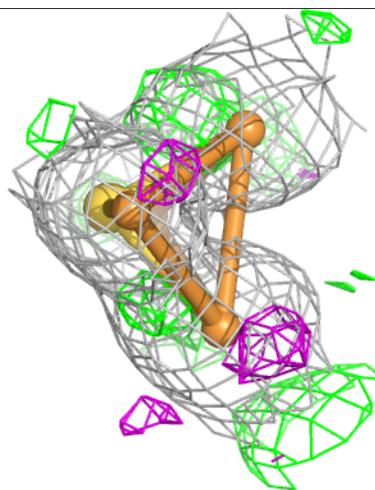
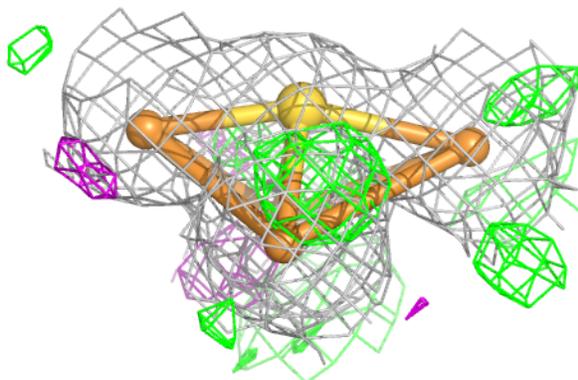
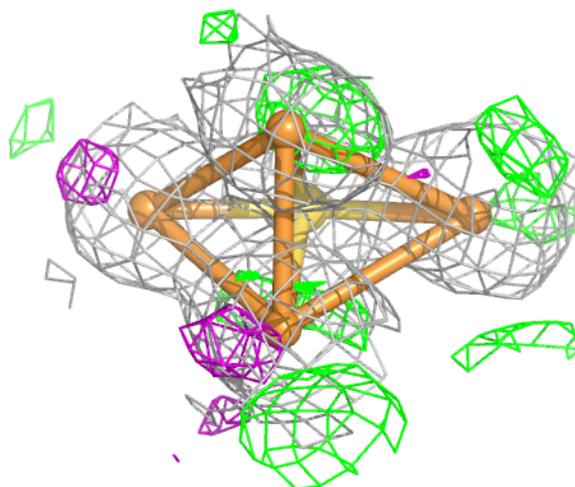
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	FMT	A	712	3/3	0.59	0.25	55,55,63,64	0
6	FMT	B	2201	3/3	0.62	0.26	64,65,78,79	0
6	FMT	A	707	3/3	0.64	0.15	64,64,67,68	0
6	FMT	A	714	3/3	0.66	0.24	59,59,63,64	0
6	FMT	A	705	3/3	0.68	0.14	58,58,61,63	0
6	FMT	A	715	3/3	0.75	0.13	57,57,59,59	0
6	FMT	A	718	3/3	0.83	0.22	47,49,59,65	0
6	FMT	A	717	3/3	0.84	0.14	64,67,80,81	0
2	B3P	A	701	19/19	0.87	0.12	25,33,42,43	0
6	FMT	A	716	3/3	0.88	0.25	54,54,55,56	0
6	FMT	A	706	3/3	0.91	0.14	29,29,51,57	0
2	B3P	B	2202	19/19	0.91	0.09	25,29,35,35	0
6	FMT	B	2206	3/3	0.92	0.19	45,45,46,54	0
10	TRS	A	711	8/8	0.92	0.14	35,39,45,48	0
5	K	A	704	1/1	0.93	0.08	23,23,23,23	1
6	FMT	A	713	3/3	0.94	0.14	24,24,44,53	0
6	FMT	B	2211	3/3	0.95	0.14	22,22,32,43	0
8	CUZ	B	2209	5/5	0.95	0.07	24,25,31,34	5
9	CUA	A	710	2/2	0.95	0.08	22,22,22,35	2
8	CUZ	A	709	5/5	0.96	0.10	10,24,37,50	5
9	CUA	B	2210	2/2	0.96	0.07	25,25,25,52	2
6	FMT	B	2207	3/3	0.97	0.12	21,21,42,43	0
4	CA	A	703	1/1	0.99	0.07	16,16,16,16	1
5	K	B	2205	1/1	0.99	0.09	15,15,15,15	1
4	CA	B	2204	1/1	0.99	0.07	25,25,25,25	1
7	CL	A	708	1/1	0.99	0.08	19,19,19,19	1
3	NA	B	2203	1/1	0.99	0.05	24,24,24,24	1
3	NA	A	702	1/1	1.00	0.06	16,16,16,16	1
7	CL	B	2208	1/1	1.00	0.07	27,27,27,27	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.

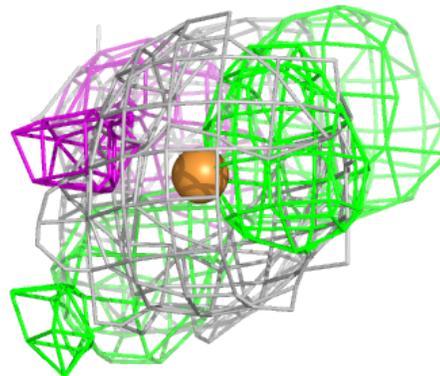
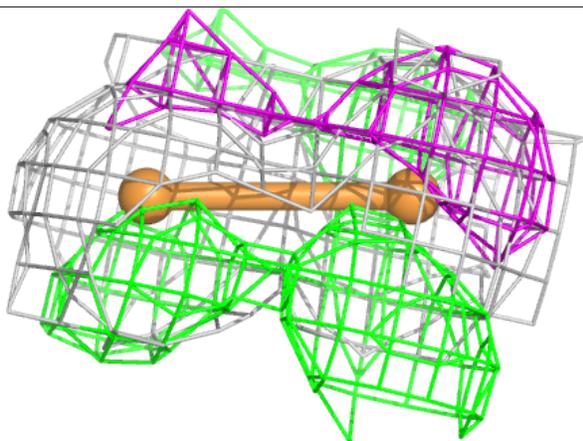
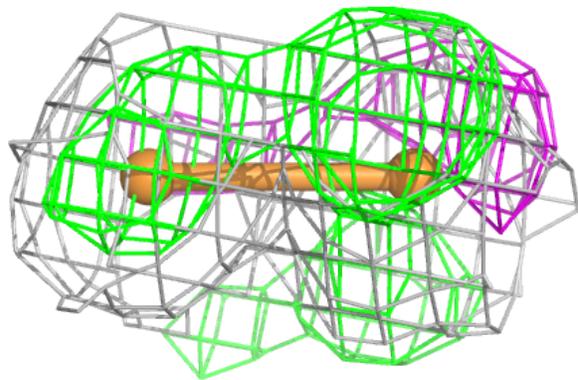
Electron density around CUZ B 2209:

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



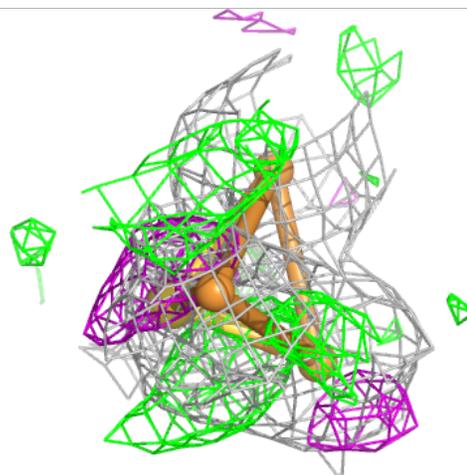
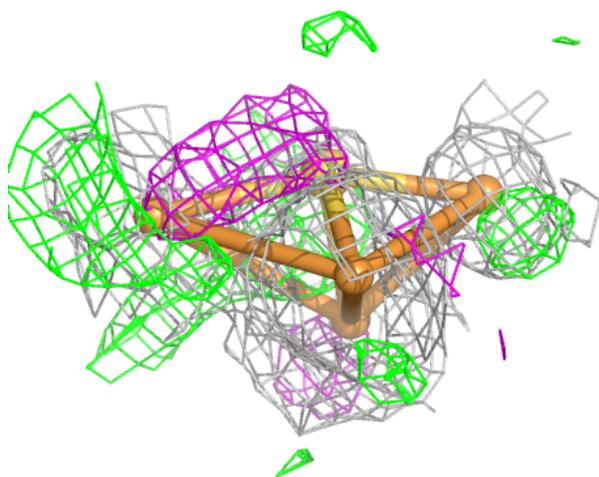
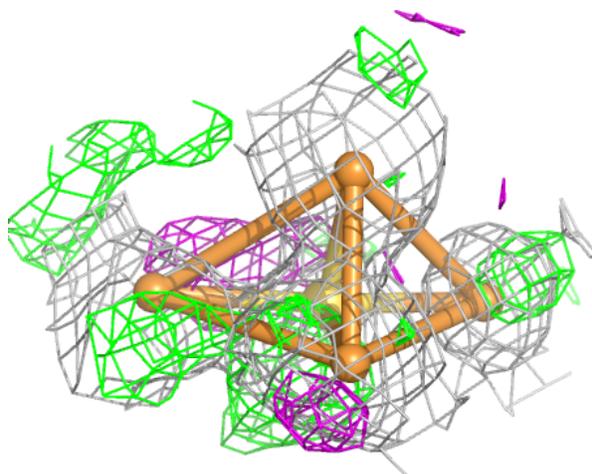
Electron density around CUA A 710:

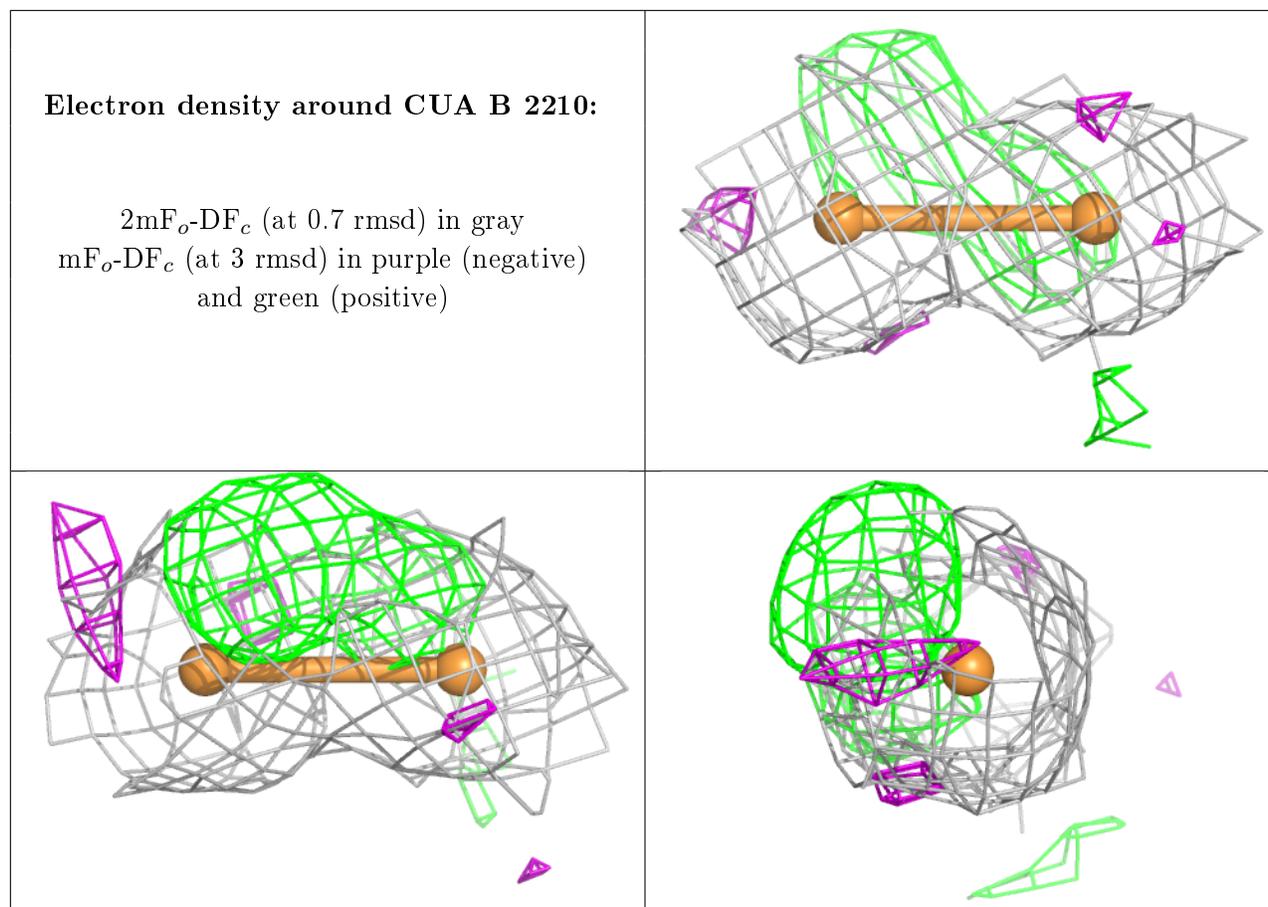
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CUZ A 709:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.