



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:33 PM UTC

PDB ID : 7Q2U / pdb_00007q2u
Title : The crystal structure of the HINT1 Q62A mutant.
Authors : Dolot, R.M.; Strom, A.M.; Wagner, C.R.
Deposited on : 2021-10-26
Resolution : 2.27 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

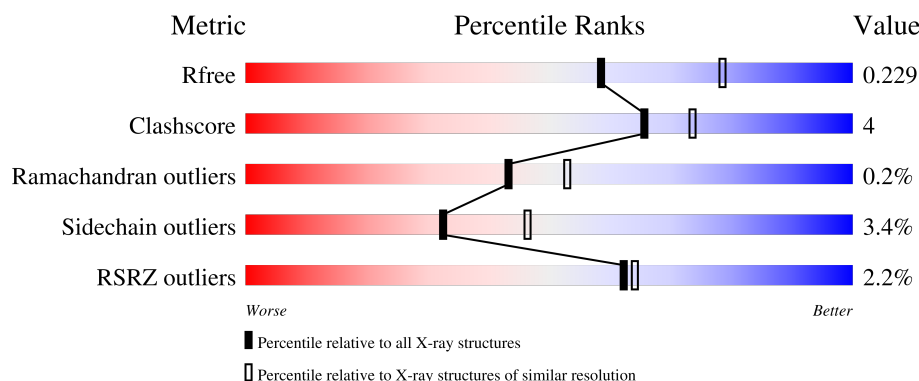
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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

Mol	Chain	Length	Quality of chain
1	AAA	126	82% 10% 8%
1	BBB	126	79% 13% 8%
1	CCC	126	83% 9% 8%
1	DDD	126	78% 13% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CAC	BBB	201	-	X	-	-
3	CAC	CCC	201	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3917 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.

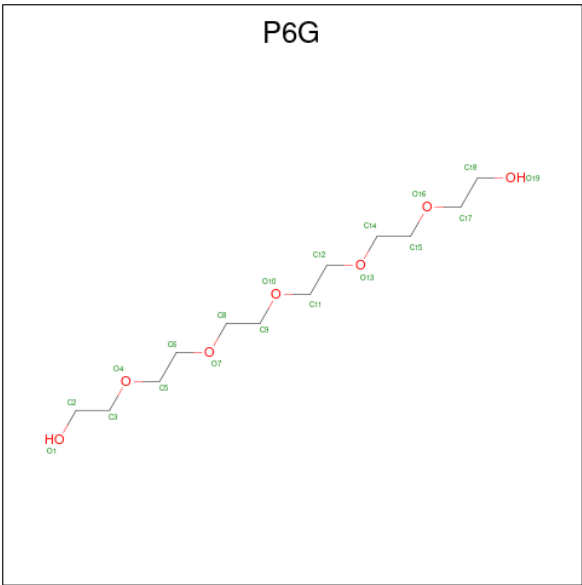
- Molecule 1 is a protein called Histidine triad nucleotide-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	116	Total	C	N	O	S	0	2	0
			907	574	163	165	5			
1	BBB	116	Total	C	N	O	S	0	2	0
			912	578	166	162	6			
1	CCC	116	Total	C	N	O	S	0	0	0
			893	567	161	160	5			
1	DDD	116	Total	C	N	O	S	0	2	0
			907	574	163	165	5			

There are 4 discrepancies between the modelled and reference sequences:

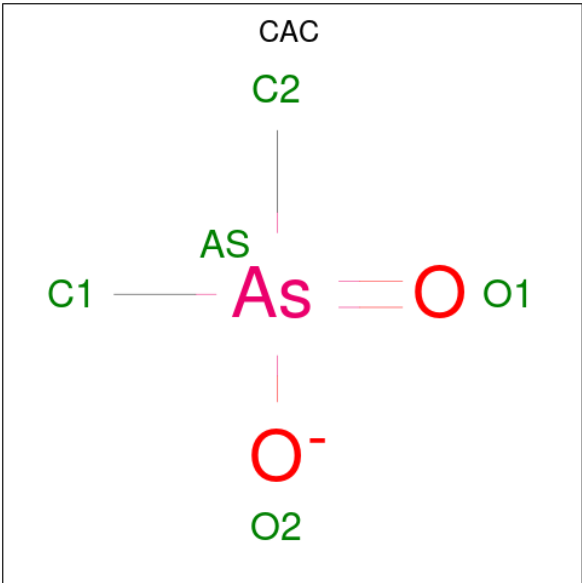
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	62	ALA	GLN	engineered mutation	UNP P49773
BBB	62	ALA	GLN	engineered mutation	UNP P49773
CCC	62	ALA	GLN	engineered mutation	UNP P49773
DDD	62	ALA	GLN	engineered mutation	UNP P49773

- Molecule 2 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇) (labeled as "Ligand of Interest" by depositor).



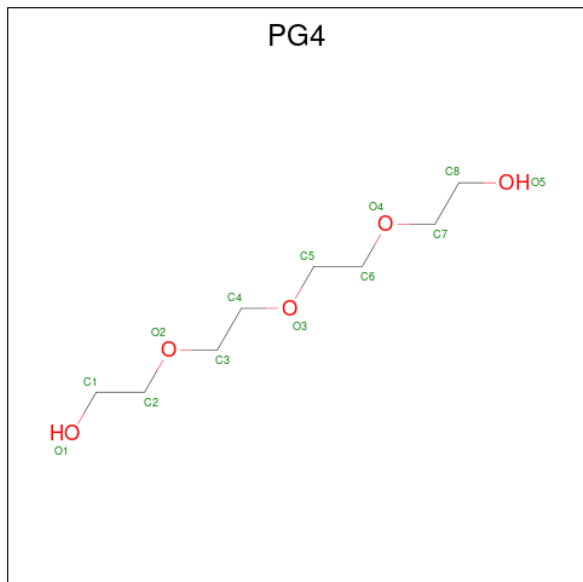
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	O		0	0
			19	12	7			

- Molecule 3 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	BBB	1	Total	As	C	O	0	0
			5	1	2	2		
3	CCC	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	DDD	1	Total	C	O	0	0
			13	8	5		

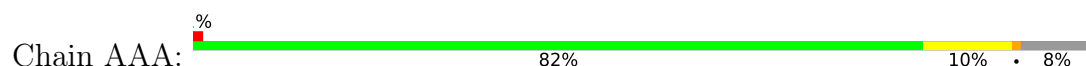
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	69	Total	O	0	0
			69	69		
5	BBB	63	Total	O	0	0
			63	63		
5	CCC	64	Total	O	0	0
			64	64		
5	DDD	60	Total	O	0	0
			60	60		

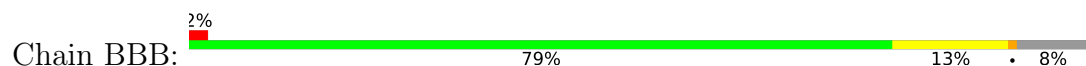
3 Residue-property plots [i](#)

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.

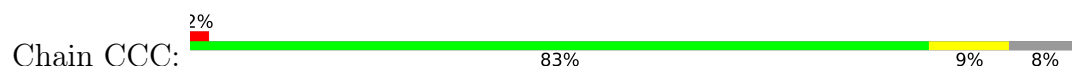
- Molecule 1: Histidine triad nucleotide-binding protein 1



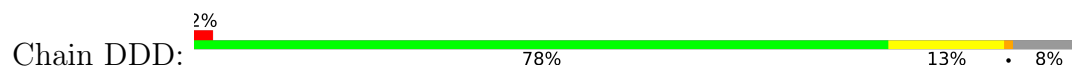
- Molecule 1: Histidine triad nucleotide-binding protein 1



- Molecule 1: Histidine triad nucleotide-binding protein 1



- Molecule 1: Histidine triad nucleotide-binding protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	112.89Å 112.89Å 43.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.73 – 2.27 40.73 – 2.27	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.73-2.27) 100.0 (40.73-2.27)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.164 , 0.220 0.172 , 0.229	Depositor DCC
R_{free} test set	1305 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3917	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: CAC, P6G, PG4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AAA	1.19	0/929	1.40	2/1253 (0.2%)
1	BBB	1.21	0/934	1.36	1/1259 (0.1%)
1	CCC	1.23	3/915 (0.3%)	1.37	0/1234
1	DDD	1.23	1/929 (0.1%)	1.43	3/1253 (0.2%)
All	All	1.21	4/3707 (0.1%)	1.39	6/4999 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	112	HIS	C-O	6.36	1.31	1.23
1	CCC	111	VAL	C-O	6.01	1.29	1.24
1	DDD	78	MET	C-O	5.61	1.30	1.24
1	CCC	114	HIS	CE1-NE2	5.55	1.38	1.32

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	35	ASP	CA-CB-CG	5.56	118.16	112.60
1	DDD	101	GLY	CA-C-N	5.37	127.93	120.63
1	DDD	101	GLY	C-N-CA	5.37	127.93	120.63
1	DDD	35	ASP	CA-CB-CG	5.25	117.85	112.60
1	AAA	101	GLY	CA-C-N	5.11	127.58	120.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	907	0	898	6	0
1	BBB	912	0	912	12	0
1	CCC	893	0	891	7	0
1	DDD	907	0	898	8	0
2	AAA	19	0	26	0	0
3	BBB	5	0	0	0	0
3	CCC	5	0	0	0	0
4	DDD	13	0	18	0	0
5	AAA	69	0	0	0	0
5	BBB	63	0	0	1	0
5	CCC	64	0	0	1	0
5	DDD	60	0	0	0	0
All	All	3917	0	3643	28	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 4.

The worst 5 of 28 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:BBB:12[A]:ARG:HG3	1:BBB:13:PRO:HD2	1.67	0.76
1:AAA:91:ASN:HD22	1:AAA:91:ASN:H	1.41	0.69
1:BBB:12[A]:ARG:CG	1:BBB:13:PRO:HD2	2.28	0.63
1:CCC:79:ILE:HG13	1:DDD:71:GLU:HG3	1.87	0.57
1:BBB:40:ALA:HA	1:BBB:53:LEU:O	2.10	0.51

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	116/126 (92%)	113 (97%)	3 (3%)	0	100	100
1	BBB	116/126 (92%)	114 (98%)	2 (2%)	0	100	100
1	CCC	114/126 (90%)	111 (97%)	3 (3%)	0	100	100
1	DDD	116/126 (92%)	109 (94%)	6 (5%)	1 (1%)	14	15
All	All	462/504 (92%)	447 (97%)	14 (3%)	1 (0%)	43	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	12	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	97/102 (95%)	93 (96%)	4 (4%)	27	38
1	BBB	97/102 (95%)	95 (98%)	2 (2%)	47	63
1	CCC	95/102 (93%)	94 (99%)	1 (1%)	65	79
1	DDD	97/102 (95%)	90 (93%)	7 (7%)	13	16
All	All	386/408 (95%)	372 (96%)	14 (4%)	32	44

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	44	ILE
1	DDD	45	SER
1	DDD	107[B]	SER
1	DDD	87	ASP
1	DDD	107[A]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands 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$
3	CAC	CCC	201	-	2,4,4	3.66	2 (100%)	4,6,6	2.78	2 (50%)
4	PG4	DDD	201	-	12,12,12	0.34	0	11,11,11	0.17	0
2	P6G	AAA	201	-	18,18,18	0.45	0	17,17,17	0.30	0
3	CAC	BBB	201	-	2,4,4	3.18	2 (100%)	4,6,6	3.08	3 (75%)

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
4	PG4	DDD	201	-	-	7/10/10/10	-
2	P6G	AAA	201	-	-	11/16/16/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	201	CAC	AS-C2	3.72	1.99	1.90
3	CCC	201	CAC	AS-C1	3.59	1.98	1.90
3	BBB	201	CAC	AS-C1	3.26	1.98	1.90
3	BBB	201	CAC	AS-C2	3.11	1.97	1.90

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	201	CAC	O2-AS-C1	4.14	115.86	105.84
3	BBB	201	CAC	O1-AS-C2	3.99	116.46	111.50
3	BBB	201	CAC	O2-AS-C1	3.98	115.48	105.84
3	CCC	201	CAC	O1-AS-C1	3.10	115.35	111.50
3	BBB	201	CAC	O1-AS-C1	-2.50	108.39	111.50

There are no chirality outliers.

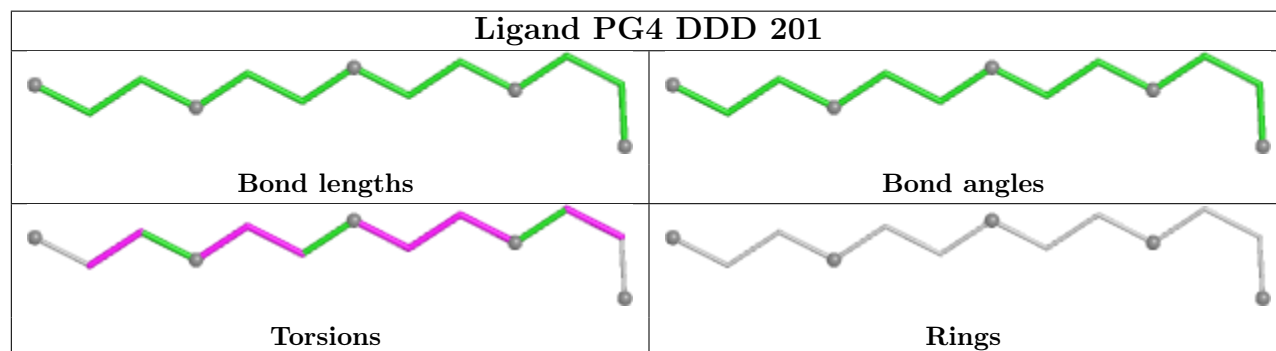
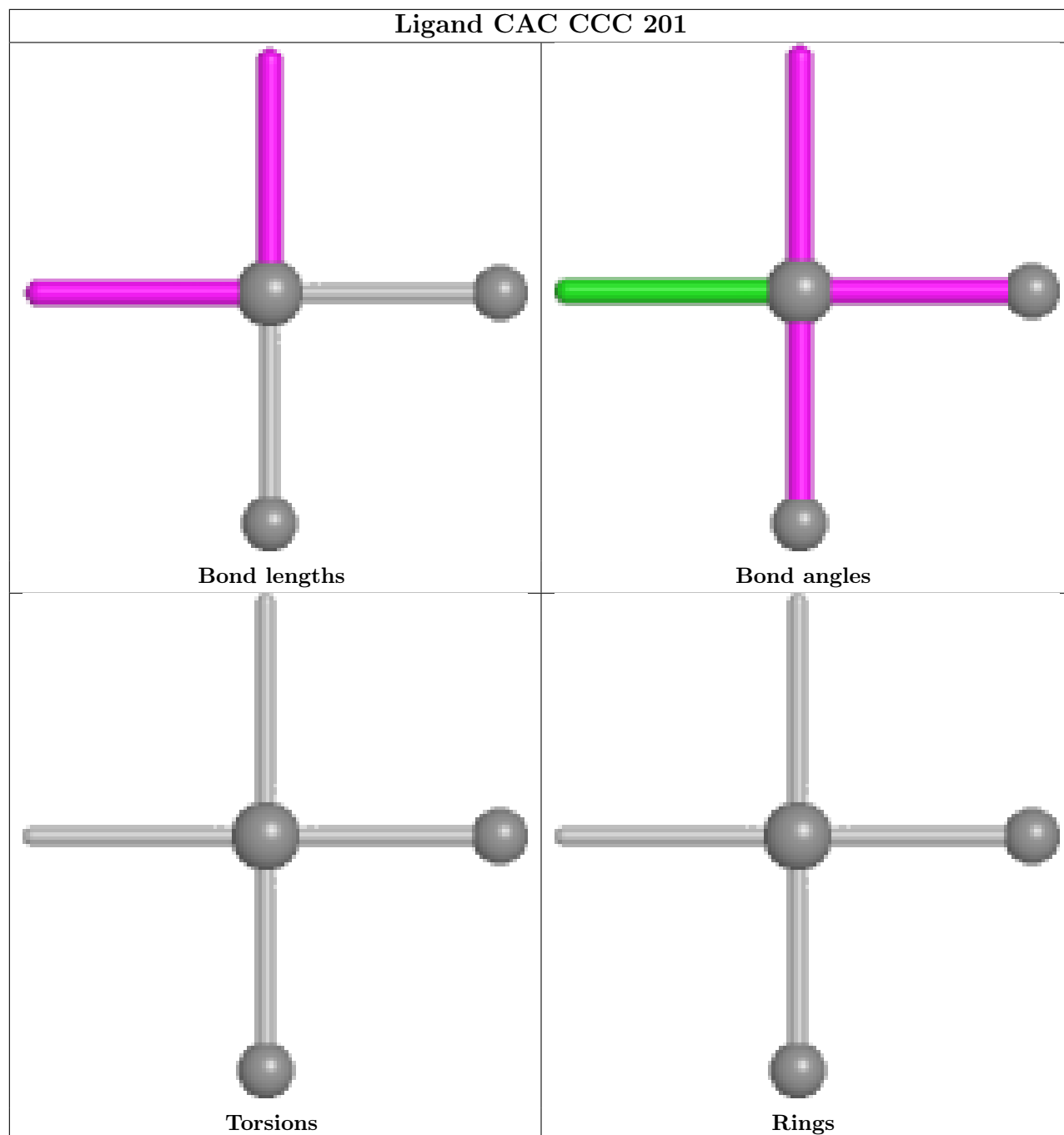
5 of 18 torsion outliers are listed below:

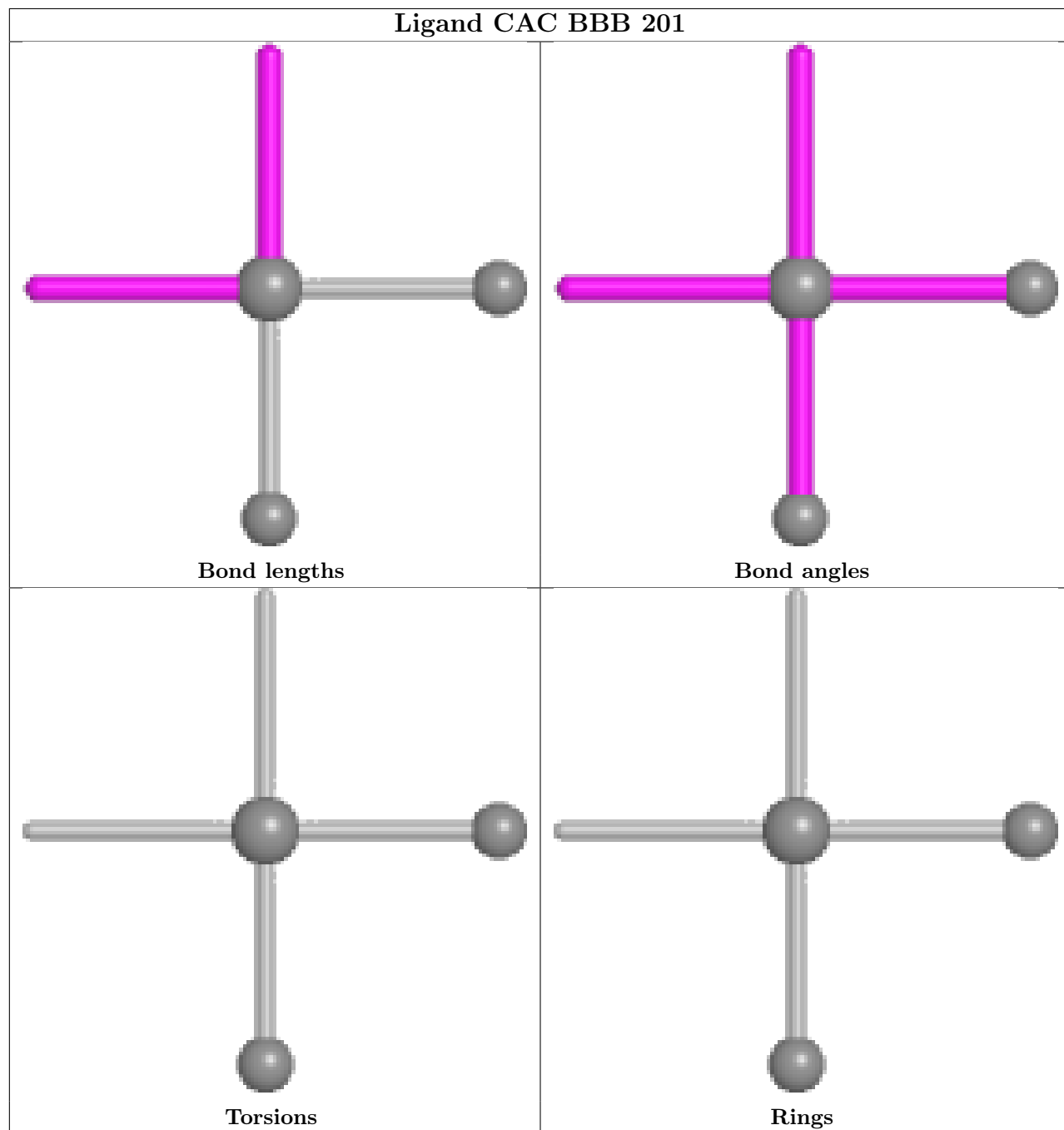
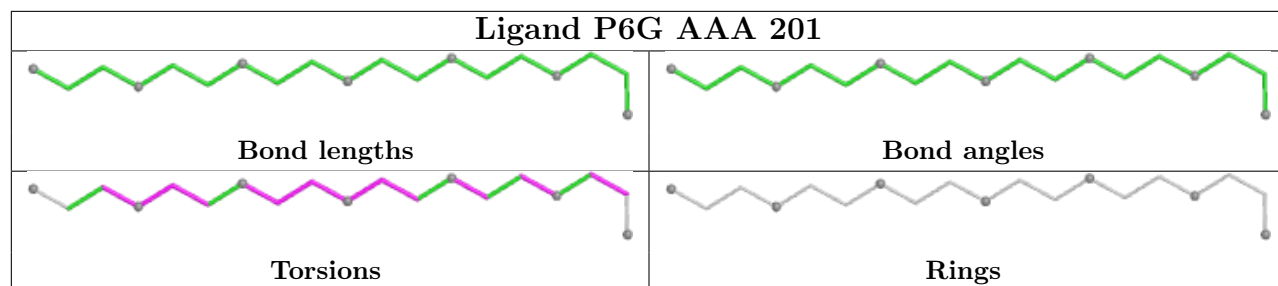
Mol	Chain	Res	Type	Atoms
4	DDD	201	PG4	O2-C3-C4-O3
4	DDD	201	PG4	O1-C1-C2-O2
4	DDD	201	PG4	O4-C7-C8-O5
2	AAA	201	P6G	O10-C11-C12-O13
2	AAA	201	P6G	C5-C6-O7-C8

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	AAA	116/126 (92%)	-0.34	1 (0%) 81 82	18, 40, 63, 130	2 (1%)
1	BBB	116/126 (92%)	-0.31	3 (2%) 57 59	20, 41, 68, 131	2 (1%)
1	CCC	116/126 (92%)	-0.22	3 (2%) 57 59	29, 42, 67, 160	0
1	DDD	116/126 (92%)	-0.16	3 (2%) 57 59	19, 45, 76, 123	2 (1%)
All	All	464/504 (92%)	-0.26	10 (2%) 62 64	18, 41, 71, 160	6 (1%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	11	ALA	4.1
1	BBB	12[A]	ARG	4.1
1	CCC	11	ALA	3.1
1	AAA	11	ALA	3.1
1	CCC	13	PRO	3.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

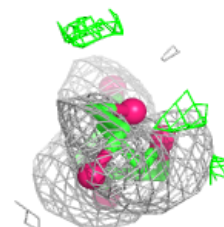
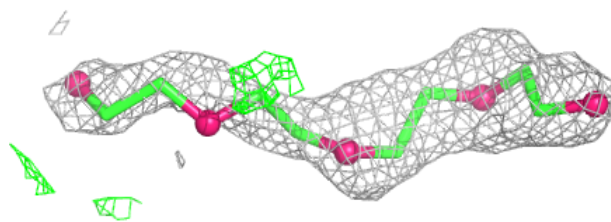
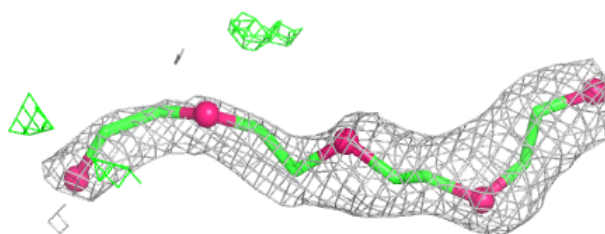
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PG4	DDD	201	13/13	0.87	0.17	72,80,102,105	0
2	P6G	AAA	201	19/19	0.88	0.14	59,70,80,81	0
3	CAC	CCC	201	5/5	0.97	0.12	46,59,61,63	0
3	CAC	BBB	201	5/5	0.98	0.12	58,59,69,70	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.

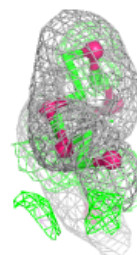
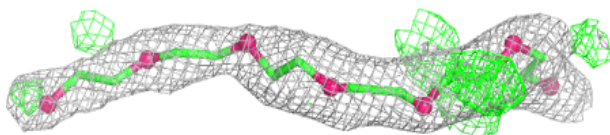
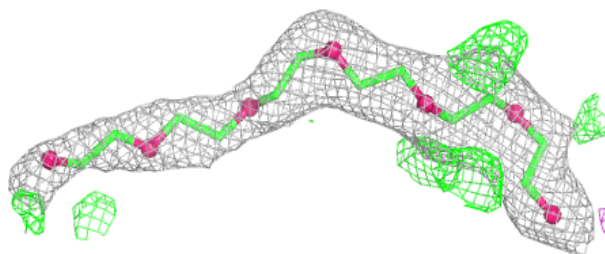
Electron density around PG4 DDD 201:

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



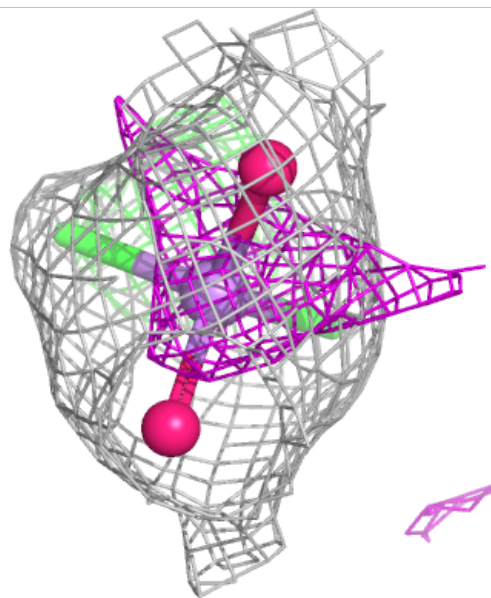
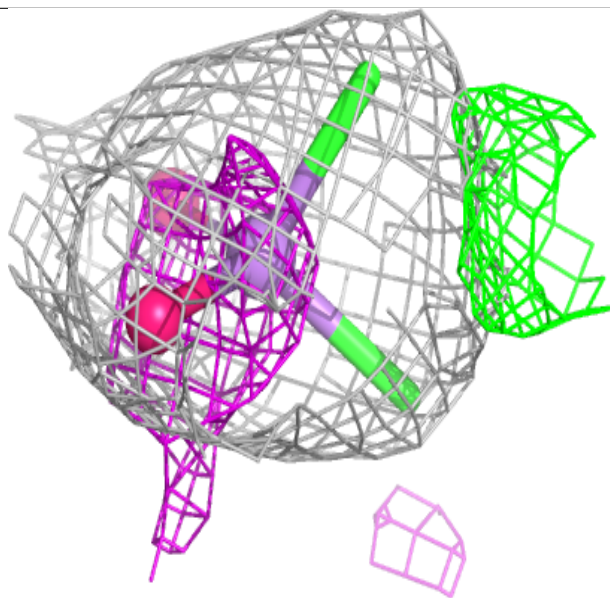
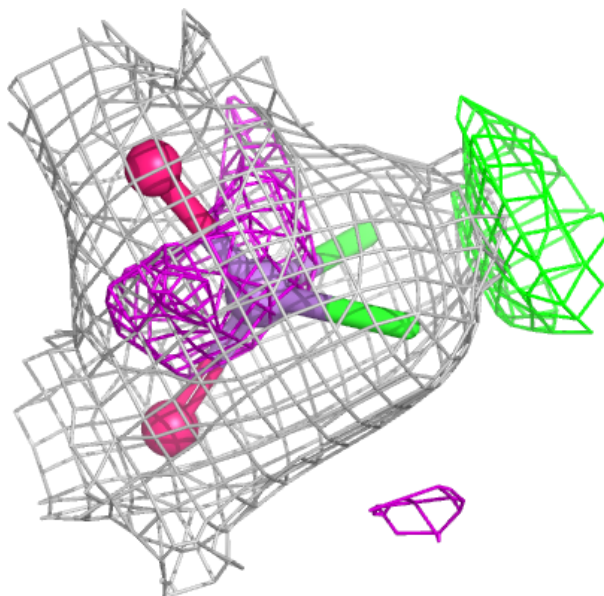
Electron density around P6G AAA 201:

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



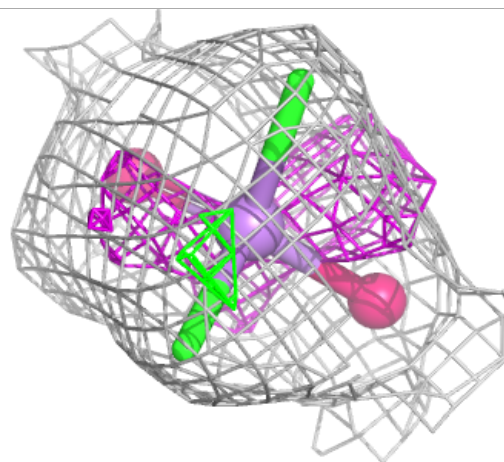
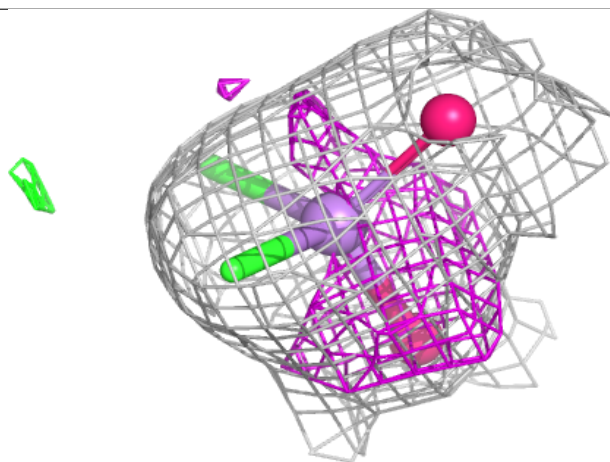
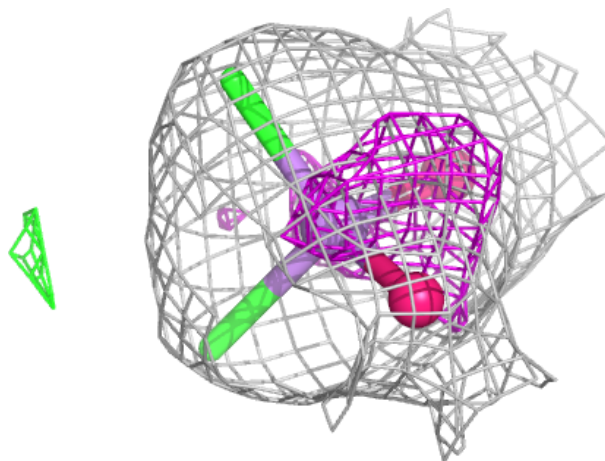
Electron density around CAC CCC 201:

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



Electron density around CAC BBB 201:

$2mF_o-DF_c$ (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.