



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:50 AM UTC

PDB ID : 8AYQ / pdb_00008ayq
Title : NaK C-DI mutant with Rb⁺ and Ca²⁺
Authors : Minniberger, S.; Plested, A.J.R.
Deposited on : 2022-09-02
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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
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

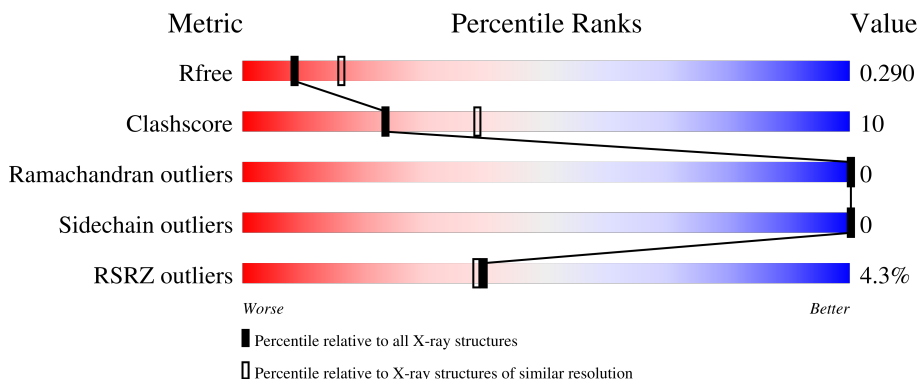
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	96	4% 73% 24% .
1	B	96	2% 74% 22% ..
1	C	96	4% 76% 21% .
1	D	96	6% 72% 26% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6322 atoms, of which 3238 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 Potassium channel protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	93	Total	C	H	N	O	S	0	0	0
			1475	487	753	106	128	1			
1	B	93	Total	C	H	N	O	S	0	0	0
			1464	487	740	108	128	1			
1	C	93	Total	C	H	N	O	S	0	0	0
			1443	480	731	105	126	1			
1	D	94	Total	C	H	N	O	S	0	0	0
			1496	497	762	109	127	1			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP Q81HW2
A	66	CYS	ASP	engineered mutation	UNP Q81HW2
A	?	-	GLY	deletion	UNP Q81HW2
A	67	ASP	ASN	engineered mutation	UNP Q81HW2
A	68	ILE	PHE	engineered mutation	UNP Q81HW2
A	110	LEU	-	expression tag	UNP Q81HW2
A	111	VAL	-	expression tag	UNP Q81HW2
A	112	PRO	-	expression tag	UNP Q81HW2
A	113	ARG	-	expression tag	UNP Q81HW2
B	18	MET	-	initiating methionine	UNP Q81HW2
B	66	CYS	ASP	engineered mutation	UNP Q81HW2
B	?	-	GLY	deletion	UNP Q81HW2
B	67	ASP	ASN	engineered mutation	UNP Q81HW2
B	68	ILE	PHE	engineered mutation	UNP Q81HW2
B	110	LEU	-	expression tag	UNP Q81HW2
B	111	VAL	-	expression tag	UNP Q81HW2
B	112	PRO	-	expression tag	UNP Q81HW2
B	113	ARG	-	expression tag	UNP Q81HW2
C	18	MET	-	initiating methionine	UNP Q81HW2
C	66	CYS	ASP	engineered mutation	UNP Q81HW2
C	?	-	GLY	deletion	UNP Q81HW2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	67	ASP	ASN	engineered mutation	UNP Q81HW2
C	68	ILE	PHE	engineered mutation	UNP Q81HW2
C	110	LEU	-	expression tag	UNP Q81HW2
C	111	VAL	-	expression tag	UNP Q81HW2
C	112	PRO	-	expression tag	UNP Q81HW2
C	113	ARG	-	expression tag	UNP Q81HW2
D	18	MET	-	initiating methionine	UNP Q81HW2
D	66	CYS	ASP	engineered mutation	UNP Q81HW2
D	?	-	GLY	deletion	UNP Q81HW2
D	67	ASP	ASN	engineered mutation	UNP Q81HW2
D	68	ILE	PHE	engineered mutation	UNP Q81HW2
D	110	LEU	-	expression tag	UNP Q81HW2
D	111	VAL	-	expression tag	UNP Q81HW2
D	112	PRO	-	expression tag	UNP Q81HW2
D	113	ARG	-	expression tag	UNP Q81HW2

- Molecule 2 is RUBIDIUM ION (CCD ID: RB) (formula: Rb) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Rb 2 2	0	0
2	C	2	Total Rb 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 3 3	0	1
3	B	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			22	6	14	2		
4	A	1	Total	C	H	O	0	0
			22	6	14	2		
4	A	1	Total	C	H	O	0	0
			22	6	14	2		
4	B	1	Total	C	H	O	0	0
			22	6	14	2		
4	B	1	Total	C	H	O	0	0
			22	6	14	2		
4	B	1	Total	C	H	O	0	0
			22	6	14	2		
4	B	1	Total	C	H	O	0	0
			22	6	14	2		
4	B	1	Total	C	H	O	0	0
			22	6	14	2		
4	B	1	Total	C	H	O	0	0
			22	6	14	2		
4	C	1	Total	C	H	O	0	0
			22	6	14	2		
4	D	1	Total	C	H	O	0	0
			22	6	14	2		
4	D	1	Total	C	H	O	0	0
			22	6	14	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	H	O	0	0
			22	6	14	2		
4	D	1	Total	C	H	O	0	0
			22	6	14	2		
4	D	1	Total	C	H	O	0	0
			22	6	14	2		
4	D	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

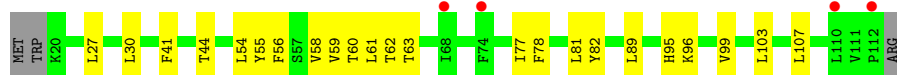
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	O	0	0
			4	4		
6	B	14	Total	O	0	0
			14	14		
6	C	8	Total	O	0	0
			8	8		
6	D	11	Total	O	0	0
			11	11		

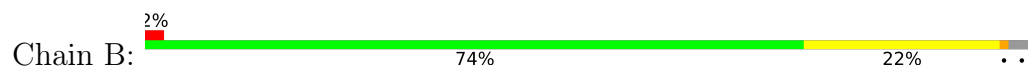
3 Residue-property plots [i](#)

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.

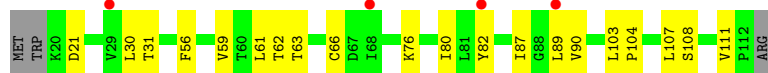
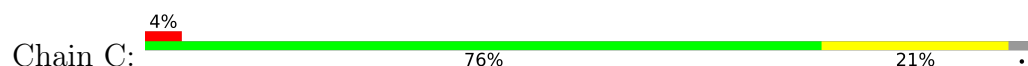
- Molecule 1: Potassium channel protein



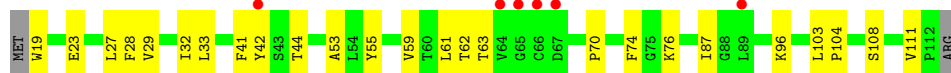
- Molecule 1: Potassium channel protein



- Molecule 1: Potassium channel protein



- Molecule 1: Potassium channel protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	67.57Å 175.51Å 67.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.78 – 2.75 33.78 – 2.75	Depositor EDS
% Data completeness (in resolution range)	93.2 (33.78-2.75) 96.2 (33.78-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.76Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.255 , 0.300 0.255 , 0.290	Depositor DCC
R_{free} test set	519 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 78.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6322	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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: CA, CL, RB, MPD

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	0.36	0/738	0.71	0/1008
1	B	0.28	0/740	0.67	1/1011 (0.1%)
1	C	0.23	0/728	0.60	0/996
1	D	0.32	0/752	0.68	0/1027
All	All	0.30	0/2958	0.67	1/4042 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	VAL	N-CA-C	5.03	119.79	109.34

There are no chirality outliers.

There are no planarity outliers.

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	722	753	753	14	0
1	B	724	740	754	17	0
1	C	712	731	732	14	0
1	D	734	762	764	17	0
2	A	2	0	0	0	0
2	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	24	42	42	0	0
4	B	64	112	112	4	0
4	C	8	14	14	1	0
4	D	48	84	84	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	4	0	0	0	0
6	B	14	0	0	1	0
6	C	8	0	0	0	0
6	D	11	0	0	0	0
All	All	3084	3238	3255	64	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 10.

All (64) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:HIS:O	1:B:99:VAL:HG23	1.82	0.78
1:D:28:PHE:CE1	1:D:32:ILE:HD11	2.23	0.74
1:D:28:PHE:CZ	1:D:32:ILE:HD11	2.26	0.70
1:C:61:LEU:O	1:C:87:ILE:HD13	1.93	0.69
1:C:108:SER:O	1:C:111:VAL:HG22	1.93	0.69
1:C:76:LYS:O	1:C:80:ILE:HD12	1.92	0.68
1:C:31:THR:HG23	1:C:90:VAL:HG22	1.77	0.66
1:D:61:LEU:O	1:D:87:ILE:HD13	1.98	0.63
1:B:27:LEU:HD12	1:B:96:LYS:HD2	1.83	0.61
1:D:108:SER:O	1:D:111:VAL:HG22	2.01	0.60
1:C:59:VAL:HG21	1:C:66:CYS:HB2	1.84	0.59
4:B:202:MPD:O4	4:B:206:MPD:H52	2.04	0.58
1:B:101:VAL:HG13	1:D:44:THR:HG21	1.85	0.57
1:A:27:LEU:HD12	1:A:96:LYS:HG3	1.88	0.56
1:B:62:THR:O	1:B:63:THR:OG1	2.23	0.55
1:A:30:LEU:HD21	1:B:106:ILE:HG13	1.89	0.55
1:B:21:ASP:OD1	1:B:22:LYS:N	2.41	0.54
1:A:77:ILE:O	1:A:81:LEU:HD13	2.08	0.53
1:D:70:PRO:HB2	1:D:76:LYS:HG2	1.91	0.52
1:D:41:PHE:C	1:D:41:PHE:CD1	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:TYR:HB2	1:D:53:ALA:HB1	1.92	0.50
1:B:113:ARG:NH1	6:B:302:HOH:O	2.31	0.50
1:C:30:LEU:HB2	1:C:89:LEU:HD11	1.93	0.50
1:B:87:ILE:HG23	1:B:88:GLY:N	2.26	0.50
1:A:62:THR:O	1:A:63:THR:OG1	2.30	0.50
1:D:29:VAL:O	1:D:33:LEU:HD23	2.12	0.49
1:B:41:PHE:CE2	1:B:45:VAL:HG21	2.47	0.49
1:B:41:PHE:CZ	1:B:45:VAL:HG21	2.47	0.49
1:C:76:LYS:O	1:C:80:ILE:CD1	2.59	0.49
1:A:55:TYR:O	1:A:59:VAL:HG22	2.12	0.48
1:D:74:PHE:HZ	4:D:206:MPD:H52	1.78	0.48
1:A:41:PHE:CZ	1:A:78:PHE:CB	2.97	0.48
1:B:41:PHE:O	1:B:45:VAL:HG22	2.14	0.48
1:C:56:PHE:HA	1:C:59:VAL:HG22	1.96	0.47
1:C:62:THR:O	1:C:63:THR:OG1	2.19	0.47
1:C:61:LEU:HD13	1:C:82:TYR:CE2	2.50	0.46
4:D:203:MPD:H32	4:D:205:MPD:HM1	1.96	0.46
1:A:103:LEU:HG	1:A:107:LEU:HD23	1.98	0.46
1:D:62:THR:O	1:D:63:THR:OG1	2.26	0.46
1:A:95:HIS:O	1:A:99:VAL:HG23	2.17	0.45
1:C:107:LEU:O	1:C:111:VAL:HG13	2.16	0.45
1:B:61:LEU:HD11	1:B:82:TYR:CZ	2.51	0.45
1:C:21:ASP:HB2	4:C:203:MPD:HM3	1.98	0.45
1:A:56:PHE:CE1	1:A:60:THR:HG21	2.52	0.45
4:B:206:MPD:O4	4:B:206:MPD:HM2	2.17	0.45
1:B:56:PHE:HA	1:B:59:VAL:HG22	1.99	0.44
1:B:55:TYR:O	1:B:59:VAL:HG22	2.17	0.44
1:A:54:LEU:O	1:A:58:VAL:HG23	2.18	0.43
1:B:103:LEU:N	1:B:104:PRO:CD	2.82	0.43
1:D:74:PHE:CZ	4:D:206:MPD:H52	2.54	0.43
1:A:44:THR:OG1	1:D:29:VAL:HG21	2.18	0.43
1:A:77:ILE:O	1:A:81:LEU:CD1	2.67	0.43
1:B:103:LEU:HB3	1:B:104:PRO:HD3	2.01	0.43
4:B:206:MPD:C1	4:B:206:MPD:H53	2.48	0.43
1:B:27:LEU:CD1	1:B:96:LYS:HD2	2.48	0.42
1:C:103:LEU:HB3	1:C:104:PRO:HD3	2.01	0.42
4:B:203:MPD:H52	4:B:203:MPD:H11	2.02	0.42
1:D:55:TYR:O	1:D:59:VAL:HG22	2.19	0.42
1:D:27:LEU:CD1	1:D:96:LYS:HG3	2.50	0.42
1:D:103:LEU:N	1:D:104:PRO:HD2	2.36	0.41
1:A:30:LEU:HD13	1:A:89:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HD11	1:A:82:TYR:CZ	2.57	0.40
1:C:30:LEU:CB	1:C:89:LEU:HD11	2.52	0.40
1:D:19:TRP:O	1:D:23:GLU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	91/96 (95%)	88 (97%)	3 (3%)	0	100	100
1	B	91/96 (95%)	89 (98%)	2 (2%)	0	100	100
1	C	91/96 (95%)	91 (100%)	0	0	100	100
1	D	92/96 (96%)	90 (98%)	2 (2%)	0	100	100
All	All	365/384 (95%)	358 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	83/87 (95%)	83 (100%)	0	100	100
1	B	83/87 (95%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	80/87 (92%)	80 (100%)	0	100	100
1	D	83/87 (95%)	83 (100%)	0	100	100
All	All	329/348 (94%)	329 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	25	GLN
1	B	100	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 11 are monoatomic - leaving 18 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	$\# Z > 2$
4	MPD	D	207	-	7,7,7	1.32	1 (14%)	9,10,10	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MPD	B	205	-	7,7,7	1.00	1 (14%)	9,10,10	0.69	0
4	MPD	B	202	-	7,7,7	0.97	0	9,10,10	0.76	0
4	MPD	D	204	-	7,7,7	1.11	0	9,10,10	0.57	0
4	MPD	D	202	-	7,7,7	0.85	0	9,10,10	0.77	0
4	MPD	D	203	-	7,7,7	0.96	0	9,10,10	0.78	0
4	MPD	B	207	-	7,7,7	0.83	0	9,10,10	0.69	0
4	MPD	D	206	-	7,7,7	0.87	0	9,10,10	0.64	0
4	MPD	B	209	-	7,7,7	0.80	0	9,10,10	0.68	0
4	MPD	D	205	-	7,7,7	0.96	1 (14%)	9,10,10	0.65	0
4	MPD	B	204	-	7,7,7	1.09	1 (14%)	9,10,10	0.83	0
4	MPD	B	208	-	7,7,7	0.91	0	9,10,10	0.75	0
4	MPD	B	206	-	7,7,7	1.24	0	9,10,10	0.50	0
4	MPD	A	206	-	7,7,7	0.93	0	9,10,10	0.79	0
4	MPD	B	203	-	7,7,7	1.14	1 (14%)	9,10,10	0.51	0
4	MPD	A	205	-	7,7,7	1.83	3 (42%)	9,10,10	0.50	0
4	MPD	A	207	-	7,7,7	1.08	1 (14%)	9,10,10	0.63	0
4	MPD	C	203	-	7,7,7	1.02	1 (14%)	9,10,10	0.70	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	D	207	-	-	0/5/5/5	-
4	MPD	B	205	-	-	0/5/5/5	-
4	MPD	B	202	-	-	1/5/5/5	-
4	MPD	D	204	-	-	2/5/5/5	-
4	MPD	D	202	-	-	1/5/5/5	-
4	MPD	D	203	-	-	2/5/5/5	-
4	MPD	B	207	-	-	1/5/5/5	-
4	MPD	D	206	-	-	2/5/5/5	-
4	MPD	B	209	-	-	2/5/5/5	-
4	MPD	D	205	-	-	1/5/5/5	-
4	MPD	B	204	-	-	2/5/5/5	-
4	MPD	B	208	-	-	1/5/5/5	-
4	MPD	B	206	-	-	3/5/5/5	-
4	MPD	A	206	-	-	2/5/5/5	-
4	MPD	B	203	-	-	3/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	A	205	-	-	3/5/5/5	-
4	MPD	A	207	-	-	3/5/5/5	-
4	MPD	C	203	-	-	1/5/5/5	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	207	MPD	O2-C2	-2.43	1.38	1.44
4	A	205	MPD	C3-C2	2.41	1.61	1.54
4	A	205	MPD	C1-C2	2.39	1.59	1.52
4	C	203	MPD	O2-C2	-2.33	1.39	1.44
4	D	205	MPD	O2-C2	-2.28	1.39	1.44
4	A	205	MPD	CM-C2	2.24	1.58	1.52
4	B	203	MPD	O2-C2	-2.22	1.39	1.44
4	B	205	MPD	O2-C2	-2.07	1.39	1.44
4	B	204	MPD	O2-C2	-2.06	1.39	1.44
4	D	207	MPD	O2-C2	-2.05	1.39	1.44

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	205	MPD	C2-C3-C4-C5
4	B	203	MPD	C2-C3-C4-O4
4	B	203	MPD	C2-C3-C4-C5
4	B	206	MPD	C2-C3-C4-C5
4	A	205	MPD	O2-C2-C3-C4
4	B	206	MPD	O2-C2-C3-C4
4	A	206	MPD	C1-C2-C3-C4
4	A	206	MPD	CM-C2-C3-C4
4	A	207	MPD	C1-C2-C3-C4
4	A	207	MPD	CM-C2-C3-C4
4	B	202	MPD	C2-C3-C4-C5
4	B	204	MPD	C2-C3-C4-C5
4	B	207	MPD	C2-C3-C4-C5
4	B	208	MPD	C2-C3-C4-C5
4	B	209	MPD	C2-C3-C4-C5
4	A	207	MPD	O2-C2-C3-C4
4	B	203	MPD	O2-C2-C3-C4
4	D	203	MPD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	D	206	MPD	O2-C2-C3-C4
4	A	205	MPD	C2-C3-C4-O4
4	B	204	MPD	C2-C3-C4-O4
4	B	206	MPD	C2-C3-C4-O4
4	B	209	MPD	C2-C3-C4-O4
4	D	202	MPD	C2-C3-C4-O4
4	D	205	MPD	C2-C3-C4-O4
4	C	203	MPD	C1-C2-C3-C4
4	D	203	MPD	C1-C2-C3-C4
4	D	204	MPD	C1-C2-C3-C4
4	D	204	MPD	CM-C2-C3-C4
4	D	206	MPD	C1-C2-C3-C4

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	MPD	1	0
4	D	203	MPD	1	0
4	D	206	MPD	2	0
4	D	205	MPD	1	0
4	B	206	MPD	3	0
4	B	203	MPD	1	0
4	C	203	MPD	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	93/96 (96%)	0.39	4 (4%)	40 38	64, 81, 140, 183	0
1	B	93/96 (96%)	0.34	2 (2%)	62 60	62, 87, 156, 196	0
1	C	93/96 (96%)	0.49	4 (4%)	40 38	71, 96, 128, 155	0
1	D	94/96 (97%)	0.37	6 (6%)	25 25	67, 93, 136, 141	0
All	All	373/384 (97%)	0.40	16 (4%)	40 38	62, 91, 142, 196	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	89	LEU	3.1
1	C	68	ILE	3.1
1	B	103	LEU	3.0
1	D	89	LEU	2.8
1	D	67	ASP	2.7
1	D	42	TYR	2.7
1	A	74	PHE	2.6
1	C	82	TYR	2.5
1	A	110	LEU	2.4
1	D	64	VAL	2.3
1	A	68	ILE	2.3
1	D	65	GLY	2.3
1	C	29	VAL	2.2
1	A	112	PRO	2.1
1	B	101	VAL	2.1
1	D	66	CYS	2.0

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 ⓘ

There are no oligosaccharides 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, 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.

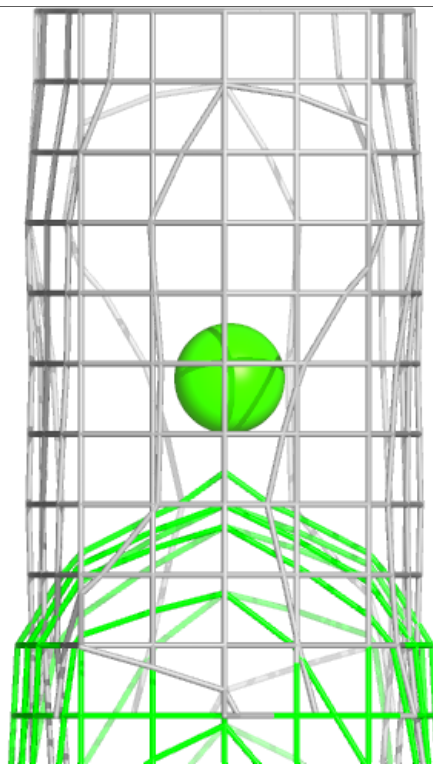
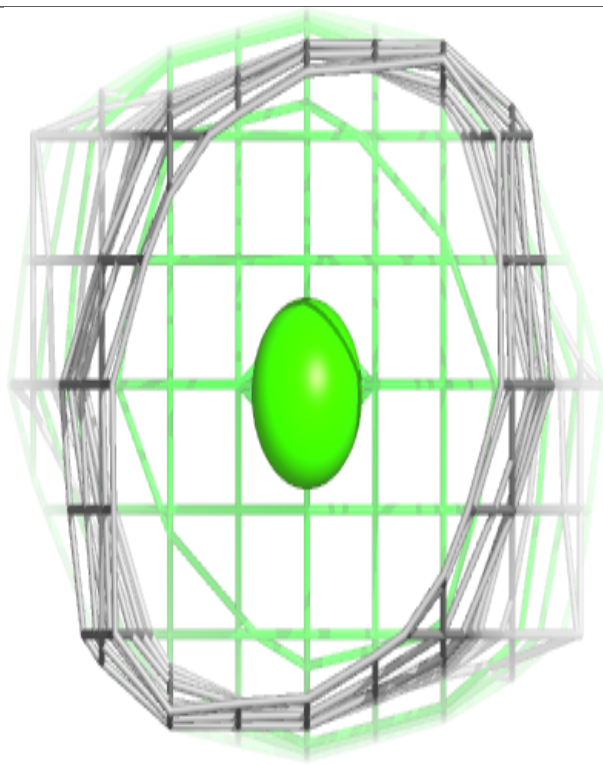
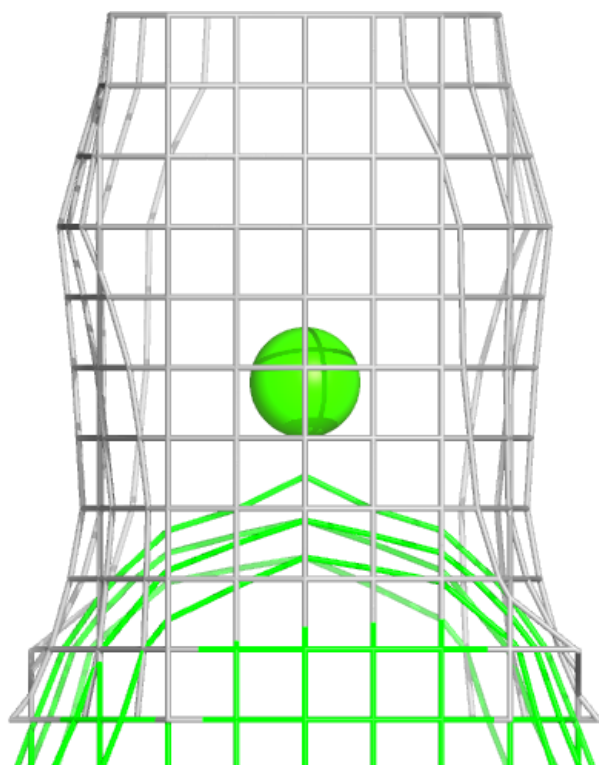
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MPD	B	209	8/8	0.43	0.13	115,139,149,151	0
4	MPD	C	203	8/8	0.43	0.15	87,112,130,138	0
4	MPD	B	206	8/8	0.58	0.14	90,115,141,141	0
4	MPD	D	206	8/8	0.68	0.19	106,130,148,163	0
4	MPD	A	206	8/8	0.71	0.14	116,143,155,172	0
4	MPD	D	204	8/8	0.72	0.14	104,126,148,148	0
3	CA	A	203	1/1	0.72	0.28	144,144,144,144	1
3	CA	D	201	1/1	0.75	0.39	140,140,140,140	1
4	MPD	B	208	8/8	0.76	0.10	91,112,132,134	0
4	MPD	D	203	8/8	0.77	0.14	86,106,123,125	0
4	MPD	D	205	8/8	0.78	0.10	98,120,144,144	0
4	MPD	D	202	8/8	0.81	0.12	94,113,118,119	0
5	CL	A	208	1/1	0.81	0.09	85,85,85,85	0
4	MPD	D	207	8/8	0.83	0.18	79,97,108,119	0
4	MPD	B	202	8/8	0.85	0.11	93,116,127,140	0
4	MPD	B	207	8/8	0.85	0.09	91,121,135,135	0
4	MPD	B	205	8/8	0.85	0.14	80,96,108,114	0
4	MPD	A	205	8/8	0.86	0.16	70,89,107,108	0
2	RB	C	201	1/1	0.86	0.13	121,121,121,121	1
4	MPD	B	203	8/8	0.87	0.14	88,109,113,119	0
4	MPD	B	204	8/8	0.88	0.12	88,109,112,112	0
4	MPD	A	207	8/8	0.88	0.12	78,94,102,105	0
2	RB	A	202	1/1	0.90	0.10	62,62,62,62	1
5	CL	B	210	1/1	0.91	0.08	61,61,61,61	0
3	CA	B	201	1/1	0.93	0.32	109,109,109,109	1
3	CA	A	204[A]	1/1	0.95	0.07	97,97,97,97	1
3	CA	A	204[B]	1/1	0.95	0.07	92,92,92,92	1
2	RB	A	201	1/1	0.96	0.04	54,54,54,54	1
2	RB	C	202	1/1	0.98	0.06	66,66,66,66	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.

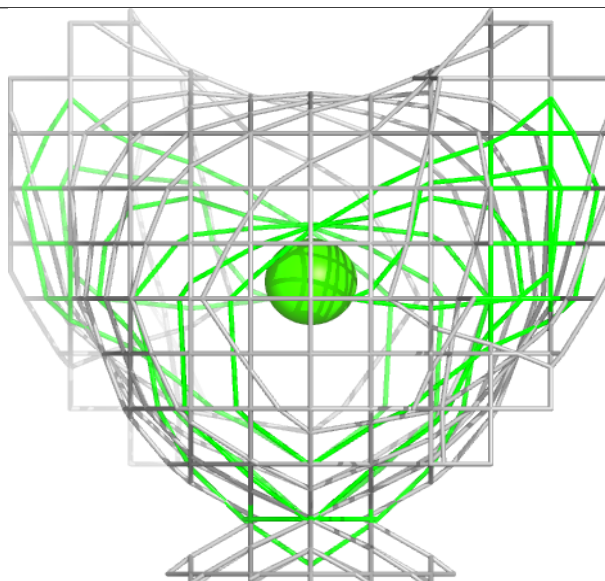
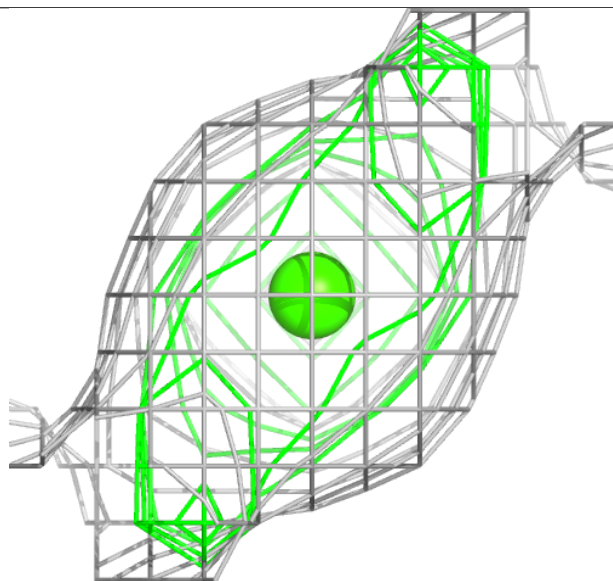
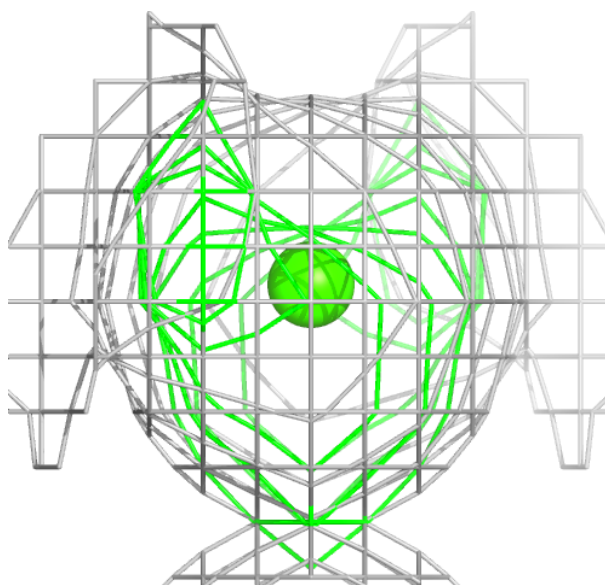
Electron density around CA A 203:

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



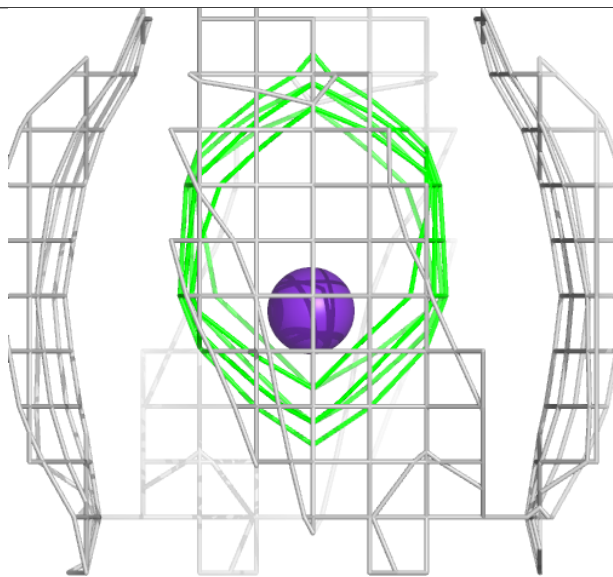
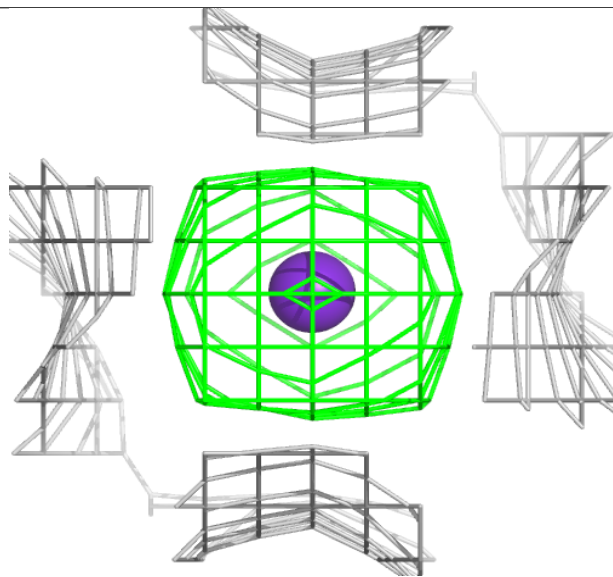
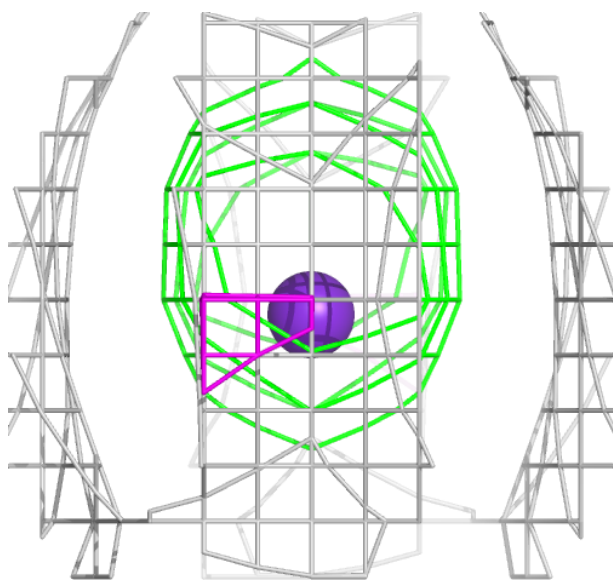
Electron density around CA D 201:

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



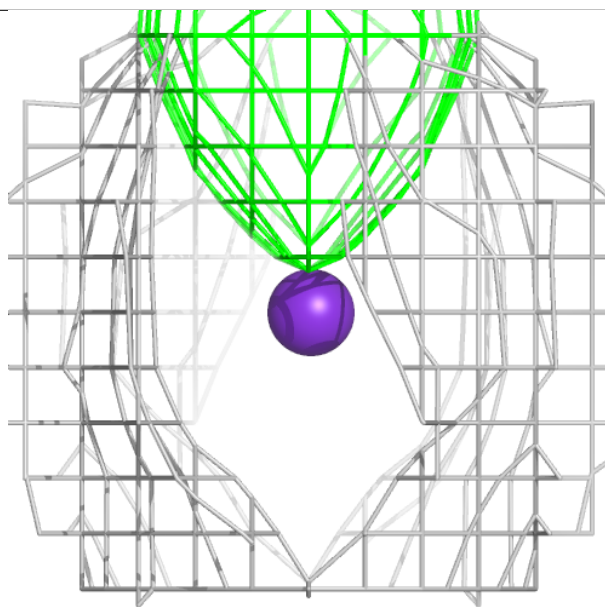
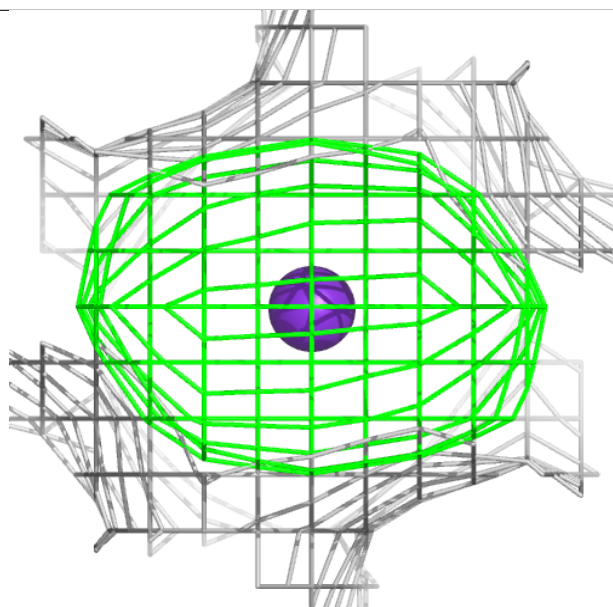
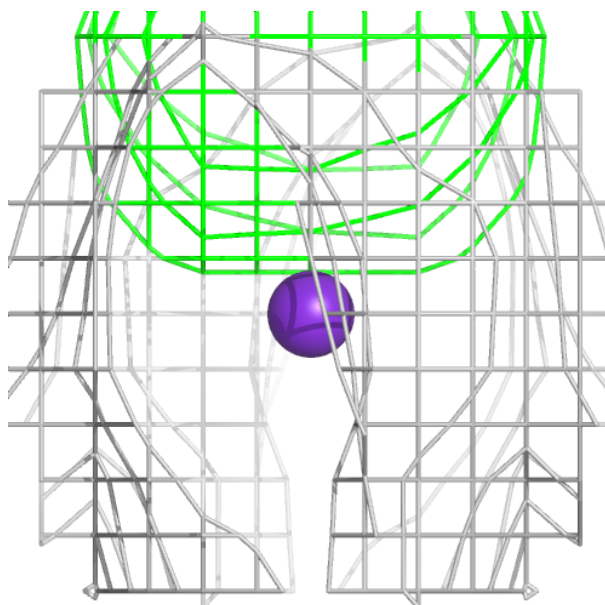
Electron density around RB C 201:

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



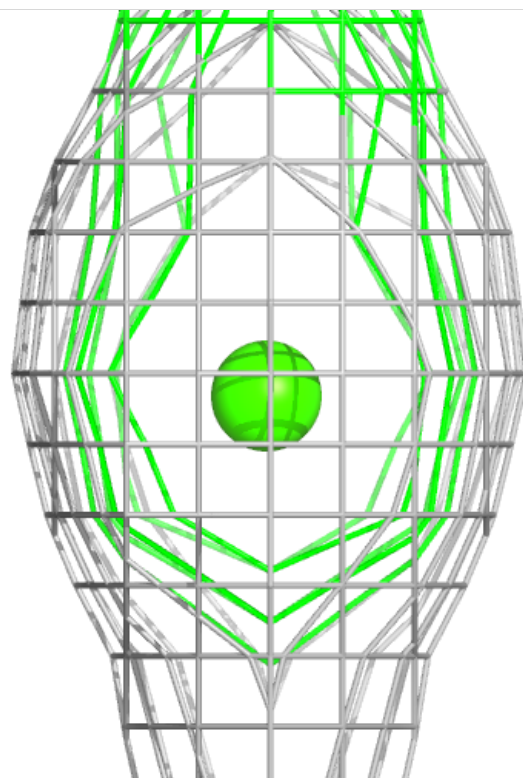
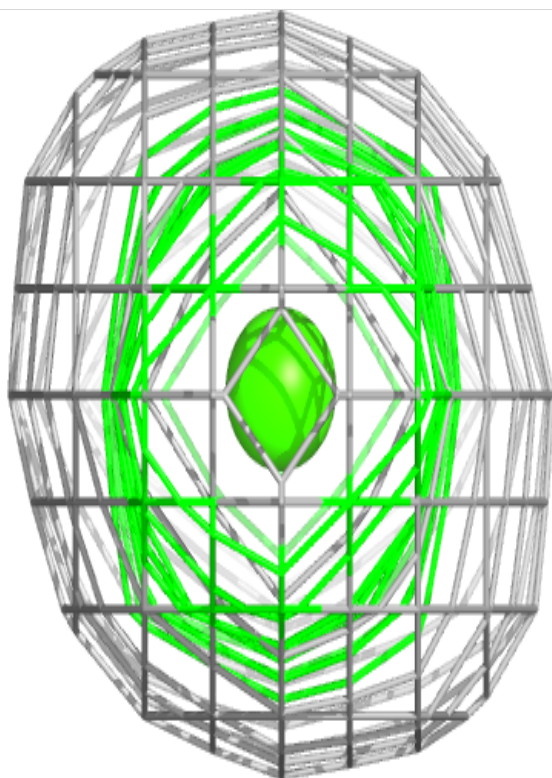
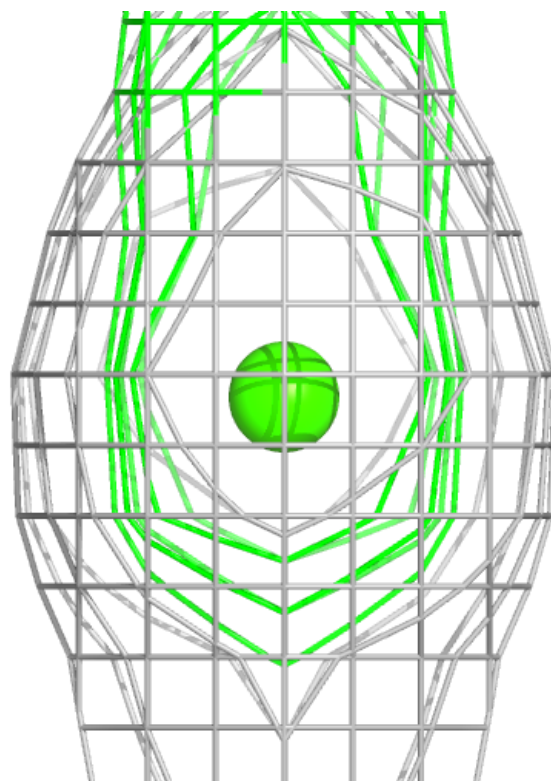
Electron density around RB A 202:

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



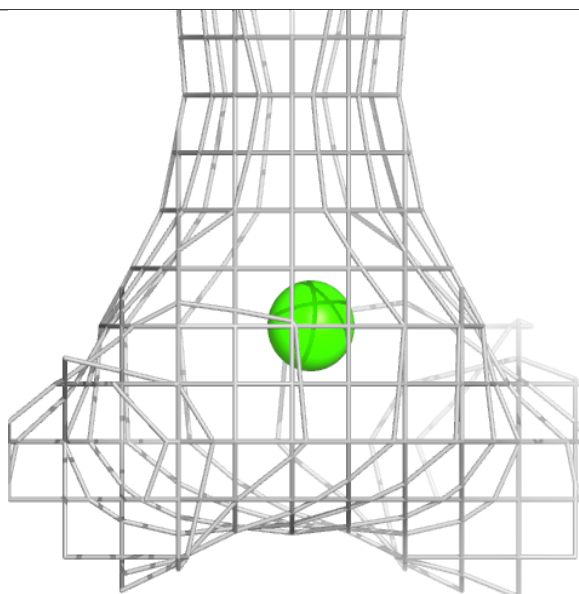
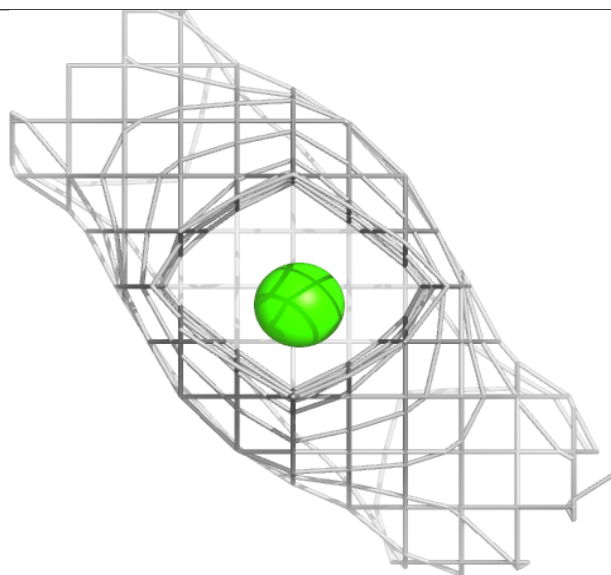
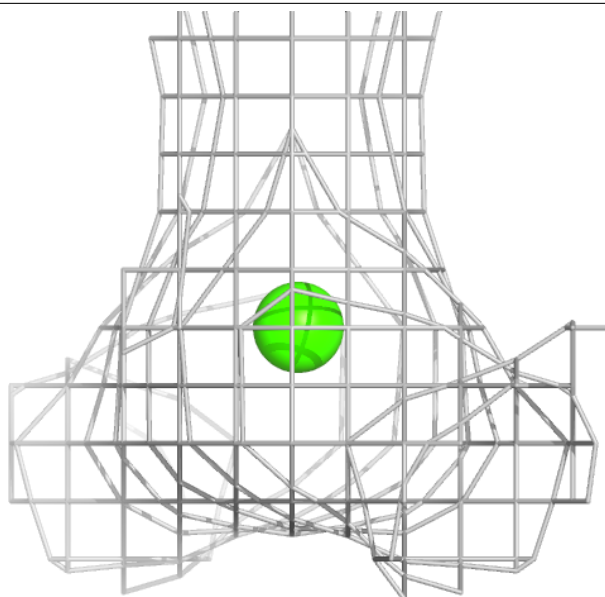
Electron density around CA B 201:

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



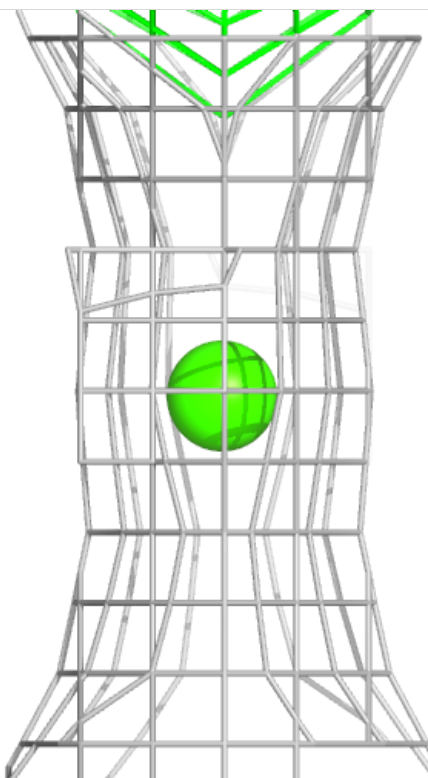
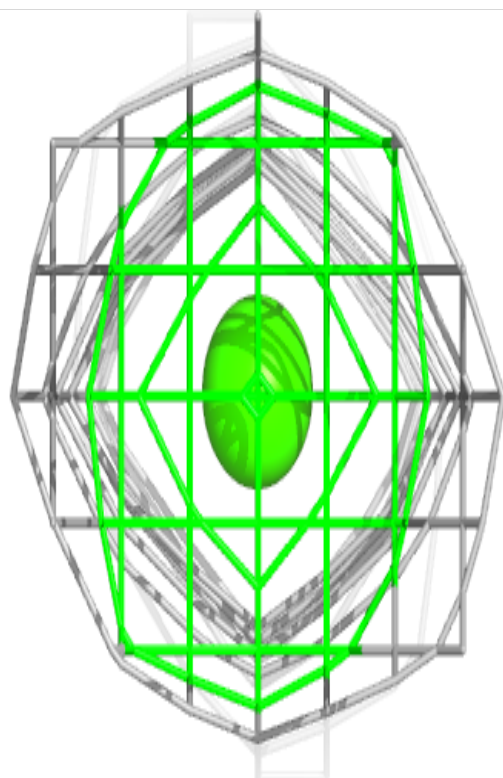
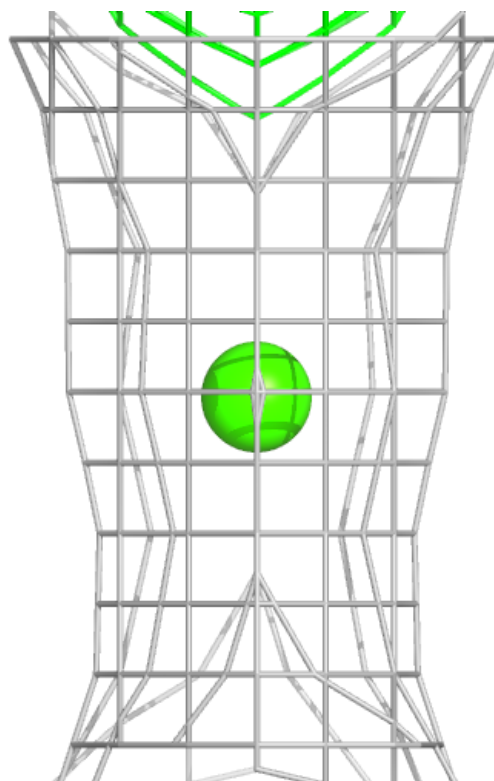
Electron density around CA A 204 (A):

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



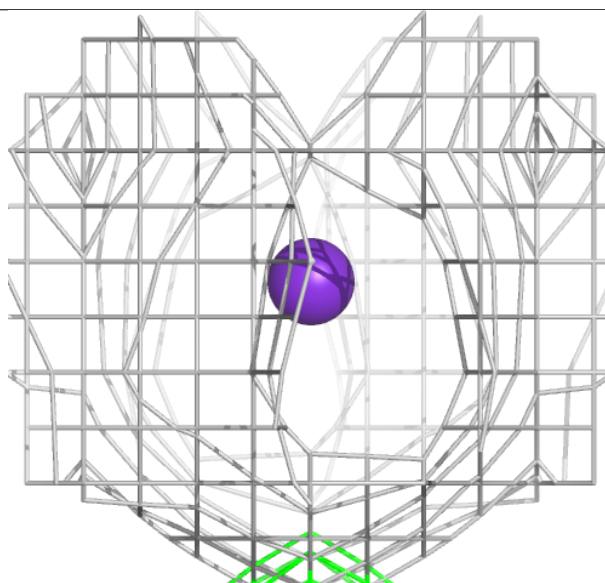
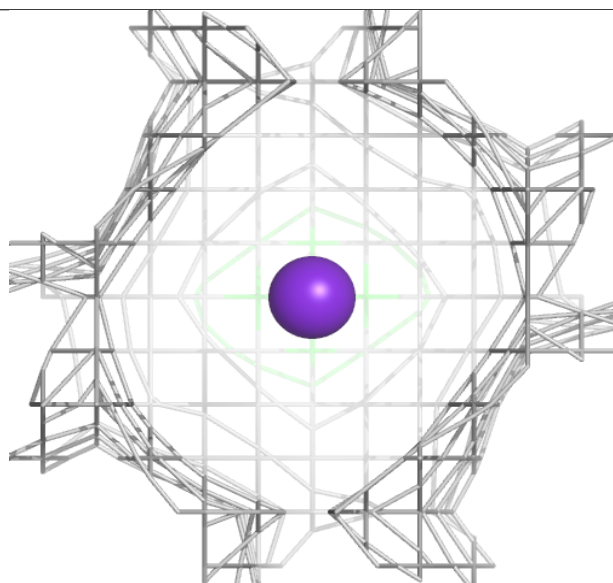
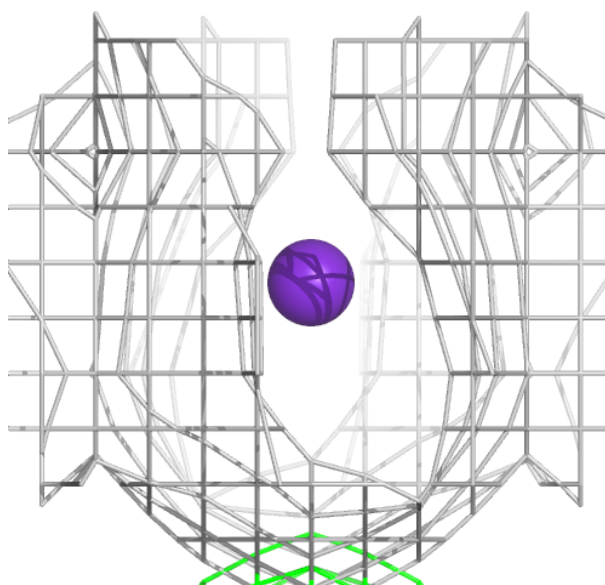
Electron density around CA A 204 (B):

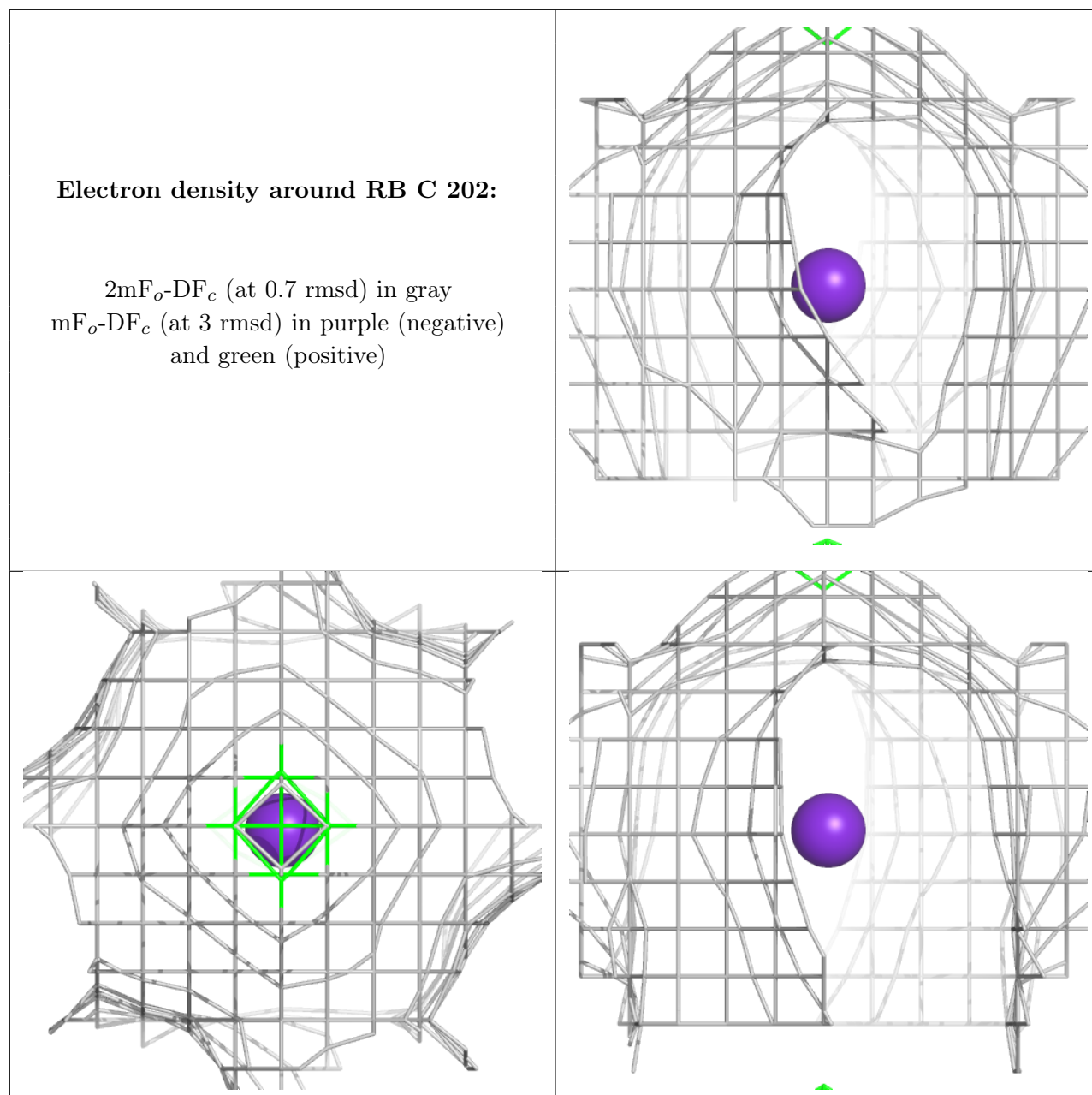
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around RB A 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 ⓘ

There are no such residues in this entry.