WORLDWIDE wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 20, 2023 – 07:12 AM EDT

PDB ID	:	5KLB
Title	:	Crystal structure of the CavAb voltage-gated calcium channel(wild-type, 2.7A)
Authors	:	Tang, L.; Gamal EL-Din, T.M.; Swanson, T.M.; Pryde, D.C.; Scheuer, T.; Zheng, N.; Catterall, W.A.
Deposited on	:	2016-06-23
Resolution	:	2.70 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

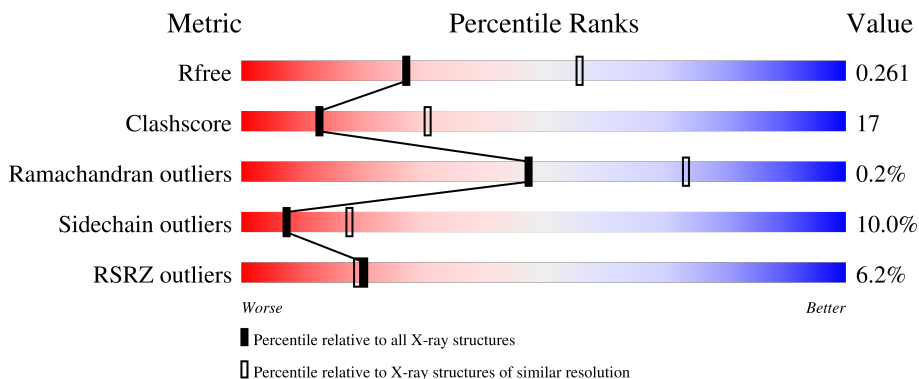|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.70 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	Percentile Ranks	Value
Rfree		0.261
Clashscore		17
Ramachandran outliers		0.2%
Sidechain outliers		10.0%
RSRZ outliers		6.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	285	4% / 64% / 25% / 5% / 6%
1	B	285	6% / 67% / 21% / 5% / 6%
1	C	285	9% / 71% / 20% / • / 6%
1	D	285	4% / 66% / 21% / 6% / 6%

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
4	CPS	A	1304	-	X	X	-
4	CPS	A	1305	-	-	X	-
4	CPS	A	1306	-	X	-	-
4	CPS	B	1307	-	X	-	-
4	CPS	B	1308	-	X	X	-
4	CPS	D	1308	-	X	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 9684 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 Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2195	1472	337	375	11			
1	B	267	Total	C	N	O	S	0	0	0
			2195	1472	337	375	11			
1	C	267	Total	C	N	O	S	0	0	0
			2195	1472	337	375	11			
1	D	267	Total	C	N	O	S	0	0	0
			2195	1472	337	375	11			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	983	MET	-	initiating methionine	UNP A8EVM5
A	984	ASP	-	expression tag	UNP A8EVM5
A	985	TYR	-	expression tag	UNP A8EVM5
A	986	LYS	-	expression tag	UNP A8EVM5
A	987	ASP	-	expression tag	UNP A8EVM5
A	988	ASP	-	expression tag	UNP A8EVM5
A	989	ASP	-	expression tag	UNP A8EVM5
A	990	ASP	-	expression tag	UNP A8EVM5
A	991	LYS	-	expression tag	UNP A8EVM5
A	992	GLY	-	expression tag	UNP A8EVM5
A	993	SER	-	expression tag	UNP A8EVM5
A	994	LEU	-	expression tag	UNP A8EVM5
A	995	VAL	-	expression tag	UNP A8EVM5
A	996	PRO	-	expression tag	UNP A8EVM5
A	997	ARG	-	expression tag	UNP A8EVM5
A	998	GLY	-	expression tag	UNP A8EVM5
A	999	SER	-	expression tag	UNP A8EVM5
A	1000	HIS	-	expression tag	UNP A8EVM5
A	1177	ASP	GLU	conflict	UNP A8EVM5
A	1178	ASP	SER	conflict	UNP A8EVM5
A	1181	ASN	MET	conflict	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	983	MET	-	initiating methionine	UNP A8EVM5
B	984	ASP	-	expression tag	UNP A8EVM5
B	985	TYR	-	expression tag	UNP A8EVM5
B	986	LYS	-	expression tag	UNP A8EVM5
B	987	ASP	-	expression tag	UNP A8EVM5
B	988	ASP	-	expression tag	UNP A8EVM5
B	989	ASP	-	expression tag	UNP A8EVM5
B	990	ASP	-	expression tag	UNP A8EVM5
B	991	LYS	-	expression tag	UNP A8EVM5
B	992	GLY	-	expression tag	UNP A8EVM5
B	993	SER	-	expression tag	UNP A8EVM5
B	994	LEU	-	expression tag	UNP A8EVM5
B	995	VAL	-	expression tag	UNP A8EVM5
B	996	PRO	-	expression tag	UNP A8EVM5
B	997	ARG	-	expression tag	UNP A8EVM5
B	998	GLY	-	expression tag	UNP A8EVM5
B	999	SER	-	expression tag	UNP A8EVM5
B	1000	HIS	-	expression tag	UNP A8EVM5
B	1177	ASP	GLU	conflict	UNP A8EVM5
B	1178	ASP	SER	conflict	UNP A8EVM5
B	1181	ASN	MET	conflict	UNP A8EVM5
C	983	MET	-	initiating methionine	UNP A8EVM5
C	984	ASP	-	expression tag	UNP A8EVM5
C	985	TYR	-	expression tag	UNP A8EVM5
C	986	LYS	-	expression tag	UNP A8EVM5
C	987	ASP	-	expression tag	UNP A8EVM5
C	988	ASP	-	expression tag	UNP A8EVM5
C	989	ASP	-	expression tag	UNP A8EVM5
C	990	ASP	-	expression tag	UNP A8EVM5
C	991	LYS	-	expression tag	UNP A8EVM5
C	992	GLY	-	expression tag	UNP A8EVM5
C	993	SER	-	expression tag	UNP A8EVM5
C	994	LEU	-	expression tag	UNP A8EVM5
C	995	VAL	-	expression tag	UNP A8EVM5
C	996	PRO	-	expression tag	UNP A8EVM5
C	997	ARG	-	expression tag	UNP A8EVM5
C	998	GLY	-	expression tag	UNP A8EVM5
C	999	SER	-	expression tag	UNP A8EVM5
C	1000	HIS	-	expression tag	UNP A8EVM5
C	1177	ASP	GLU	conflict	UNP A8EVM5
C	1178	ASP	SER	conflict	UNP A8EVM5
C	1181	ASN	MET	conflict	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	983	MET	-	initiating methionine	UNP A8EVM5
D	984	ASP	-	expression tag	UNP A8EVM5
D	985	TYR	-	expression tag	UNP A8EVM5
D	986	LYS	-	expression tag	UNP A8EVM5
D	987	ASP	-	expression tag	UNP A8EVM5
D	988	ASP	-	expression tag	UNP A8EVM5
D	989	ASP	-	expression tag	UNP A8EVM5
D	990	ASP	-	expression tag	UNP A8EVM5
D	991	LYS	-	expression tag	UNP A8EVM5
D	992	GLY	-	expression tag	UNP A8EVM5
D	993	SER	-	expression tag	UNP A8EVM5
D	994	LEU	-	expression tag	UNP A8EVM5
D	995	VAL	-	expression tag	UNP A8EVM5
D	996	PRO	-	expression tag	UNP A8EVM5
D	997	ARG	-	expression tag	UNP A8EVM5
D	998	GLY	-	expression tag	UNP A8EVM5
D	999	SER	-	expression tag	UNP A8EVM5
D	1000	HIS	-	expression tag	UNP A8EVM5
D	1177	ASP	GLU	conflict	UNP A8EVM5
D	1178	ASP	SER	conflict	UNP A8EVM5
D	1181	ASN	MET	conflict	UNP A8EVM5

- Molecule 2 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: MC3) (formula: $C_{36}H_{72}NO_8P$).

MC3
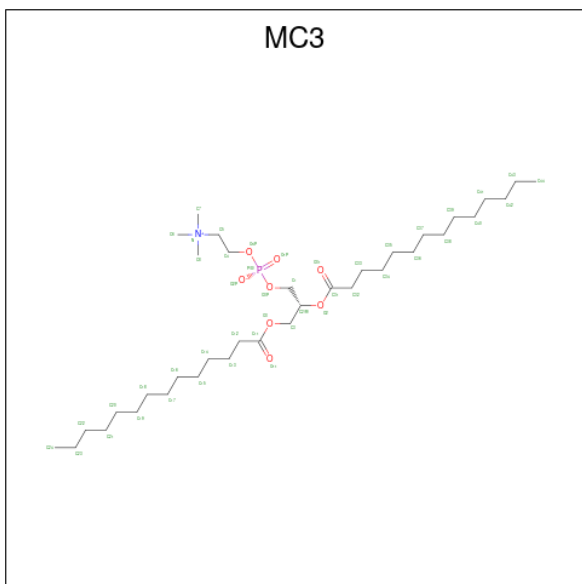
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 21 13 7 1	0	0
2	A	1	Total C N O P 46 36 1 8 1	0	0
2	B	1	Total C O P 21 13 7 1	0	0
2	B	1	Total C O P 41 32 8 1	0	0
2	B	1	Total C N O P 41 31 1 8 1	0	0
2	B	1	Total C N O P 46 36 1 8 1	0	0
2	B	1	Total C 8 8	0	0
2	C	1	Total C O P 21 13 7 1	0	0
2	C	1	Total C O P 41 32 8 1	0	0
2	C	1	Total C N O P 40 30 1 8 1	0	0
2	C	1	Total C N O P 46 36 1 8 1	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C O P 41 32 8 1	0	0
2	D	1	Total C O P 21 13 7 1	0	0
2	D	1	Total C O P 41 32 8 1	0	0
2	D	1	Total C N O P 43 33 1 8 1	0	0
2	D	1	Total C N O P 42 32 1 8 1	0	0
2	D	1	Total C N O P 46 36 1 8 1	0	0
2	D	1	Total C 8 8	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).

CPS
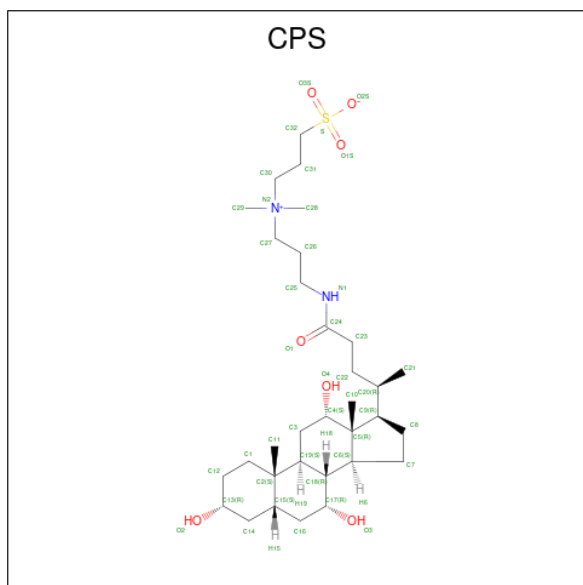
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 42	C 32	N 2	O 7	S 1	0	0
4	A	1	Total 42	C 32	N 2	O 7	S 1	0	0
4	A	1	Total 42	C 32	N 2	O 7	S 1	0	0
4	B	1	Total 42	C 32	N 2	O 7	S 1	0	0
4	B	1	Total 42	C 32	N 2	O 7	S 1	0	0
4	D	1	Total 42	C 32	N 2	O 7	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	O 3	0	0
5	B	6	Total 6	O 6	0	0
5	C	3	Total 3	O 3	0	0
5	D	5	Total 5	O 5	0	0

3 Residue-property plots ⓘ

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: Ion transport protein
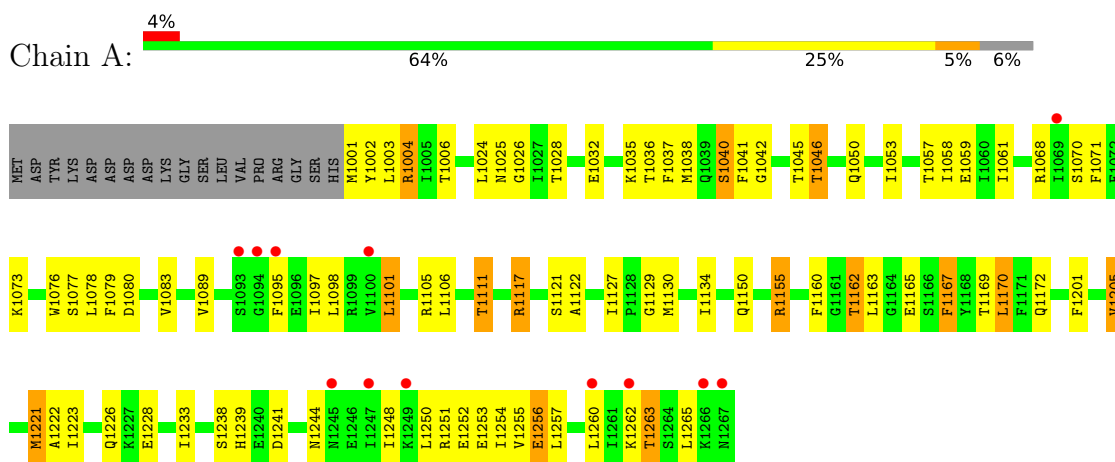
• Molecule 1: Ion transport protein

• Molecule 1: Ion transport protein

• Molecule 1: Ion transport protein

Chain D:
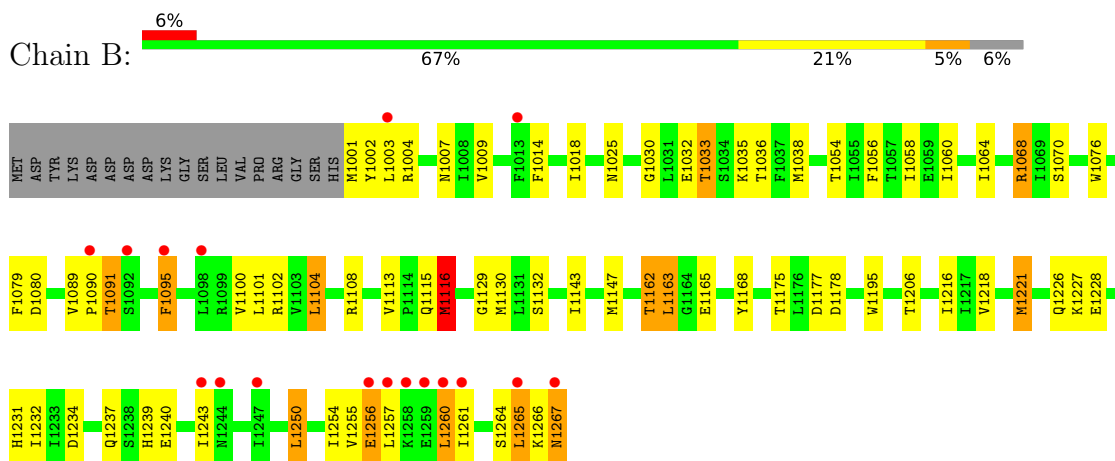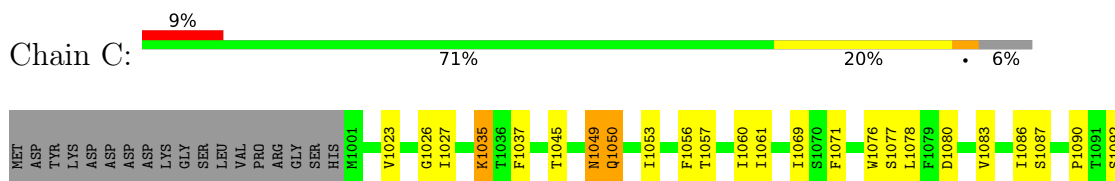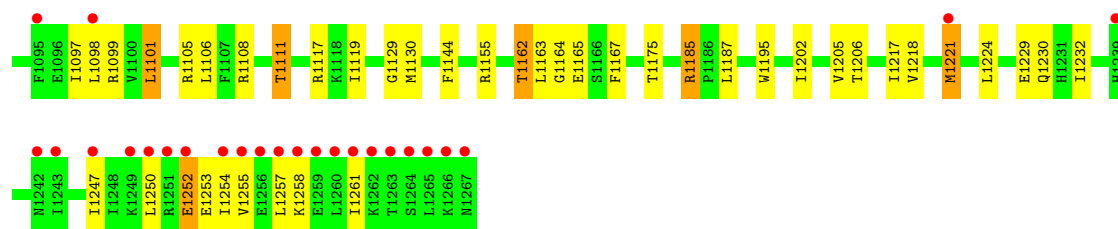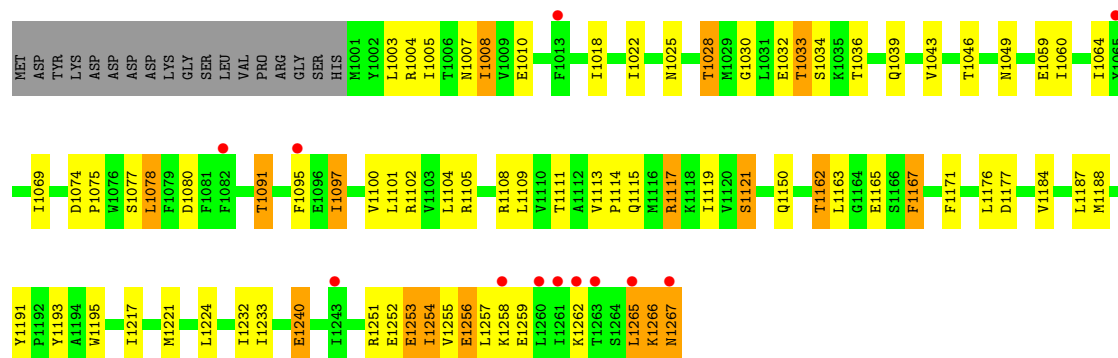
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	124.90Å 125.70Å 191.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 2.70 29.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.5 (29.93-2.70) 91.8 (29.93-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.68Å)	Xtriage
Refinement program	PHENIX dev_1839	Depositor
R, R_{free}	0.219 , 0.260 0.221 , 0.261	Depositor DCC
R_{free} test set	3791 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	58.8	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 56.1	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9684	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: CA, CPS, MC3

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	0.60	0/2248	0.65	0/3053
1	B	0.58	0/2248	0.63	1/3053 (0.0%)
1	C	0.58	0/2248	0.64	0/3053
1	D	0.61	0/2248	0.67	0/3053
All	All	0.59	0/8992	0.65	1/12212 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1116	MET	CG-SD-CE	-5.29	91.73	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2195	0	2274	54	0
1	B	2195	0	2274	60	0
1	C	2195	0	2274	55	0
1	D	2195	0	2274	53	0
2	A	67	0	91	4	0
2	B	157	0	218	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	207	0	291	22	0
2	D	201	0	283	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	126	0	135	65	0
4	B	84	0	89	39	0
4	D	42	0	45	23	0
5	A	3	0	0	0	0
5	B	6	0	0	0	0
5	C	3	0	0	0	0
5	D	5	0	0	1	0
All	All	9684	0	10248	329	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 17.

The worst 5 of 329 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)
4:A:1305:CPS:O3	4:A:1305:CPS:C17	1.69	1.39
4:D:1308:CPS:O3	4:D:1308:CPS:C17	1.70	1.39
4:A:1306:CPS:C17	4:A:1306:CPS:O3	1.70	1.39
4:B:1307:CPS:C17	4:B:1307:CPS:O3	1.69	1.38
4:A:1304:CPS:C4	4:A:1304:CPS:C10	2.02	1.37

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	A	265/285 (93%)	251 (95%)	14 (5%)	0	100	100
1	B	265/285 (93%)	254 (96%)	10 (4%)	1 (0%)	34	60
1	C	265/285 (93%)	254 (96%)	11 (4%)	0	100	100
1	D	265/285 (93%)	252 (95%)	12 (4%)	1 (0%)	34	60
All	All	1060/1140 (93%)	1011 (95%)	47 (4%)	2 (0%)	47	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1266	LYS
1	B	1255	VAL

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	A	248/264 (94%)	217 (88%)	31 (12%)	4	10
1	B	248/264 (94%)	226 (91%)	22 (9%)	9	22
1	C	248/264 (94%)	228 (92%)	20 (8%)	11	27
1	D	248/264 (94%)	222 (90%)	26 (10%)	7	16
All	All	992/1056 (94%)	893 (90%)	99 (10%)	7	18

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1086	ILE
1	C	1252	GLU
1	C	1101	LEU
1	C	1205	VAL
1	D	1028	THR

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 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	MC3	D	1303	-	40,40,45	1.77	6 (15%)	43,45,53	1.55	4 (9%)
2	MC3	D	1306	-	45,45,45	1.65	6 (13%)	51,53,53	1.58	5 (9%)
2	MC3	B	1306	-	7,7,45	0.69	0	6,6,53	0.24	0
2	MC3	B	1304	-	40,40,45	1.77	5 (12%)	46,48,53	1.82	5 (10%)
4	CPS	B	1307	-	45,45,45	11.42	29 (64%)	69,70,70	3.83	44 (63%)
2	MC3	B	1303	-	40,40,45	1.70	6 (15%)	43,45,53	1.62	4 (9%)
2	MC3	B	1302	-	20,20,45	1.78	3 (15%)	22,24,53	2.00	4 (18%)
2	MC3	A	1301	-	20,20,45	1.83	3 (15%)	22,24,53	1.43	2 (9%)
2	MC3	C	1306	-	8,8,45	0.62	0	7,7,53	0.43	0
4	CPS	D	1308	-	45,45,45	11.37	31 (68%)	69,70,70	3.97	43 (62%)
2	MC3	C	1305	-	8,8,45	0.72	0	7,7,53	0.35	0
2	MC3	B	1305	-	45,45,45	1.62	6 (13%)	51,53,53	1.62	5 (9%)
2	MC3	C	1301	-	20,20,45	1.79	4 (20%)	22,24,53	1.63	2 (9%)
2	MC3	D	1302	-	20,20,45	1.79	4 (20%)	22,24,53	1.68	3 (13%)
2	MC3	A	1303	-	45,45,45	1.56	5 (11%)	51,53,53	1.72	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	CPS	B	1308	-	45,45,45	11.34	30 (66%)	69,70,70	3.72	40 (57%)
2	MC3	C	1303	-	39,39,45	1.65	5 (12%)	45,47,53	1.77	7 (15%)
2	MC3	C	1307	-	40,40,45	1.73	5 (12%)	43,45,53	1.63	5 (11%)
2	MC3	C	1304	-	45,45,45	1.71	7 (15%)	51,53,53	1.66	6 (11%)
4	CPS	A	1305	-	45,45,45	11.47	31 (68%)	69,70,70	3.58	40 (57%)
2	MC3	C	1302	-	40,40,45	1.72	6 (15%)	43,45,53	1.62	4 (9%)
2	MC3	D	1305	-	41,41,45	1.67	4 (9%)	47,49,53	1.81	6 (12%)
4	CPS	A	1304	-	45,45,45	11.41	30 (66%)	69,70,70	3.66	40 (57%)
4	CPS	A	1306	-	45,45,45	11.36	29 (64%)	69,70,70	3.62	42 (60%)
2	MC3	D	1307	-	7,7,45	0.71	0	6,6,53	0.20	0
2	MC3	D	1304	-	42,42,45	1.69	5 (11%)	48,50,53	1.74	6 (12%)

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	MC3	D	1303	-	-	19/44/44/49	-
2	MC3	D	1306	-	-	20/49/49/49	-
2	MC3	B	1306	-	-	1/5/5/49	-
2	MC3	B	1304	-	-	22/44/44/49	-
4	CPS	B	1307	-	-	11/25/90/90	0/4/4/4
2	MC3	B	1303	-	-	23/44/44/49	-
2	MC3	B	1302	-	-	11/22/22/49	-
2	MC3	A	1301	-	-	10/22/22/49	-
2	MC3	C	1306	-	-	1/6/6/49	-
4	CPS	D	1308	-	-	16/25/90/90	0/4/4/4
2	MC3	C	1305	-	-	4/6/6/49	-
2	MC3	B	1305	-	-	28/49/49/49	-
2	MC3	C	1301	-	-	9/22/22/49	-
2	MC3	D	1302	-	-	10/22/22/49	-
2	MC3	A	1303	-	-	22/49/49/49	-
4	CPS	B	1308	-	-	18/25/90/90	0/4/4/4
2	MC3	C	1303	-	-	19/43/43/49	-
2	MC3	C	1307	-	-	24/44/44/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	C	1304	-	-	21/49/49/49	-
4	CPS	A	1305	-	-	2/25/90/90	0/4/4/4
2	MC3	C	1302	-	-	18/44/44/49	-
2	MC3	D	1305	-	-	21/45/45/49	-
4	CPS	A	1304	-	-	14/25/90/90	0/4/4/4
4	CPS	A	1306	-	-	14/25/90/90	0/4/4/4
2	MC3	D	1307	-	-	3/5/5/49	-
2	MC3	D	1304	-	-	20/46/46/49	-

The worst 5 of 260 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1304	CPS	C5-C4	-39.21	0.93	1.54
4	B	1308	CPS	C5-C4	-39.16	0.93	1.54
4	A	1305	CPS	C5-C4	-39.13	0.93	1.54
4	D	1308	CPS	C5-C4	-38.68	0.94	1.54
4	A	1306	CPS	C5-C4	-38.44	0.94	1.54

The worst 5 of 323 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1307	CPS	O1S-S-C32	-12.92	91.36	106.92
4	B	1307	CPS	O3S-S-C32	11.03	120.20	106.92
4	A	1304	CPS	C9-C5-C4	10.19	126.97	117.67
4	D	1308	CPS	O3S-S-C32	10.10	119.07	106.92
4	B	1307	CPS	C9-C5-C4	9.12	126.00	117.67

There are no chirality outliers.

5 of 381 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	MC3	O2-C2-C3-O3
2	A	1301	MC3	C1-O3P-P-O1P
2	A	1303	MC3	O3P-C1-C2-O2
2	A	1303	MC3	O4P-C4-C5-N
2	B	1302	MC3	C1-C2-C3-O3

There are no ring outliers.

24 monomers are involved in 171 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1303	MC3	2	0
2	D	1306	MC3	3	0
2	B	1306	MC3	1	0
2	B	1304	MC3	6	0
4	B	1307	CPS	13	0
2	B	1303	MC3	1	0
2	B	1302	MC3	2	0
2	A	1301	MC3	1	0
2	C	1306	MC3	1	0
4	D	1308	CPS	23	0
2	C	1305	MC3	2	0
2	B	1305	MC3	2	0
2	D	1302	MC3	1	0
2	A	1303	MC3	3	0
4	B	1308	CPS	26	0
2	C	1303	MC3	7	0
2	C	1307	MC3	4	0
2	C	1304	MC3	3	0
4	A	1305	CPS	25	0
2	C	1302	MC3	5	0
2	D	1305	MC3	1	0
4	A	1304	CPS	24	0
4	A	1306	CPS	16	0
2	D	1304	MC3	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 MC3 D 1303

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 D 1306

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 B 1306

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 B 1304

Bond lengths

Bond angles

Torsions

Rings

Ligand CPS B 1307

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 B 1303

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 B 1302

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 A 1301

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 C 1306

Bond lengths

Bond angles

Torsions

Rings

Ligand CPS D 1308	
Bond lengths
Bond angles
Torsions |
Rings |

Ligand MC3 C 1305	
Bond lengths
Bond angles
Torsions |
Rings |

Ligand MC3 B 1305

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 C 1301

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 D 1302

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 A 1303

Bond lengths

Bond angles

Torsions

Rings

Ligand CPS B 1308

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 C 1303

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 C 1307

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 C 1304

Bond lengths

Bond angles

Torsions

Rings

Ligand CPS A 1305

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 C 1302

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 D 1305

Bond lengths

Bond angles

Torsions

Rings

Ligand CPS A 1304

Bond lengths

Bond angles

Torsions

Rings

Ligand CPS A 1306

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 D 1307

Bond lengths

Bond angles

Torsions

Rings

Ligand MC3 D 1304

Bond lengths

Bond angles

Torsions

Rings

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, 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(Å²)	Q<0.9
1	A	267/285 (93%)	0.40	12 (4%)	33	31	33, 73, 160, 168	0
1	B	267/285 (93%)	0.48	17 (6%)	19	18	35, 69, 162, 181	0
1	C	267/285 (93%)	0.62	25 (9%)	8	6	35, 70, 180, 206	0
1	D	267/285 (93%)	0.42	12 (4%)	33	31	35, 70, 151, 164	0
All	All	1068/1140 (93%)	0.48	66 (6%)	20	19	33, 71, 161, 206	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1265	LEU	8.8
1	D	1261	ILE	7.1
1	C	1259	GLU	7.0
1	B	1258	LYS	6.9
1	C	1261	ILE	6.8

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, 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	CPS	A	1304	42/42	0.65	0.31	83,108,131,133	2
4	CPS	B	1308	42/42	0.74	0.25	90,108,122,124	2
2	MC3	D	1302	21/46	0.83	0.21	57,80,121,128	0
4	CPS	A	1306	42/42	0.85	0.21	54,77,81,83	2
4	CPS	A	1305	42/42	0.85	0.19	60,78,87,91	1
4	CPS	D	1308	42/42	0.85	0.18	53,71,78,86	2
2	MC3	C	1301	21/46	0.86	0.27	64,81,101,115	0
2	MC3	B	1302	21/46	0.89	0.14	56,78,93,104	0
2	MC3	A	1301	21/46	0.89	0.28	54,79,94,104	0
2	MC3	C	1305	9/46	0.90	0.18	42,48,60,60	0
4	CPS	B	1307	42/42	0.91	0.16	55,72,79,81	1
2	MC3	B	1306	8/46	0.91	0.21	43,47,54,60	0
2	MC3	C	1306	9/46	0.91	0.19	44,50,54,55	0
2	MC3	C	1302	41/46	0.92	0.23	50,66,89,93	0
2	MC3	C	1304	46/46	0.92	0.29	51,71,83,90	0
2	MC3	D	1307	8/46	0.92	0.16	42,49,51,54	0
3	CA	B	1301	1/1	0.92	0.53	103,103,103,103	0
2	MC3	B	1305	46/46	0.92	0.32	51,70,88,99	0
2	MC3	A	1303	46/46	0.93	0.35	52,69,84,93	0
2	MC3	D	1303	41/46	0.93	0.24	53,67,92,103	0
2	MC3	B	1303	41/46	0.94	0.21	58,68,93,98	0
2	MC3	C	1307	41/46	0.94	0.24	58,71,88,96	0
2	MC3	D	1306	46/46	0.95	0.24	54,68,77,82	0
2	MC3	D	1305	42/46	0.96	0.20	45,60,73,77	0
2	MC3	B	1304	41/46	0.96	0.21	46,60,75,77	0
2	MC3	C	1303	40/46	0.97	0.22	49,59,72,78	0
2	MC3	D	1304	43/46	0.97	0.22	44,56,70,77	0
3	CA	D	1301	1/1	0.98	0.12	70,70,70,70	0
3	CA	A	1302	1/1	0.99	0.19	79,79,79,79	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.
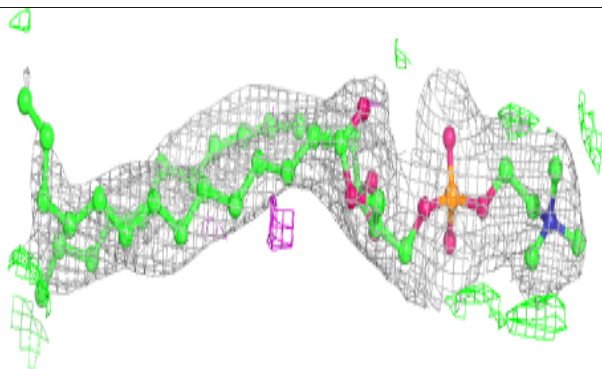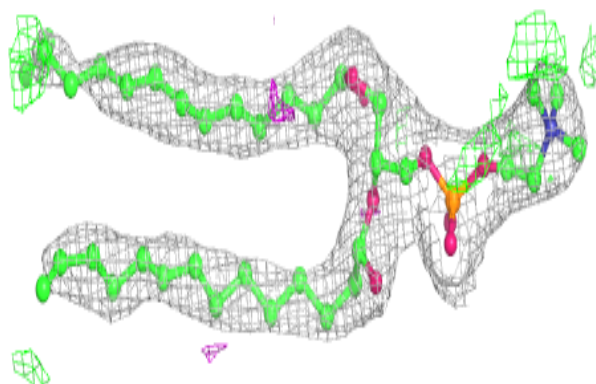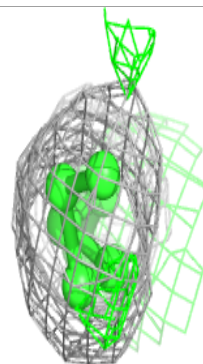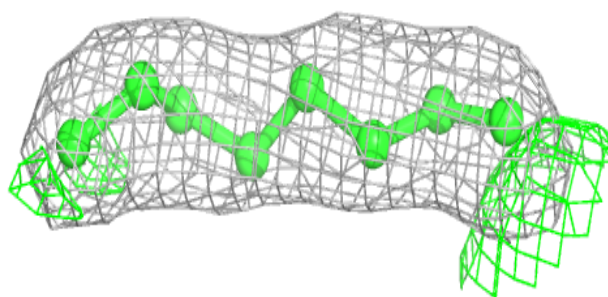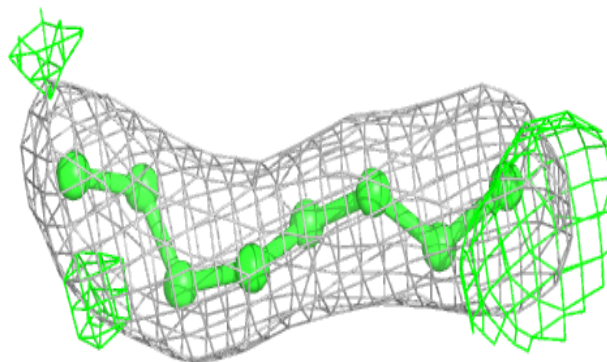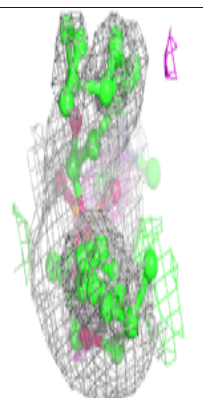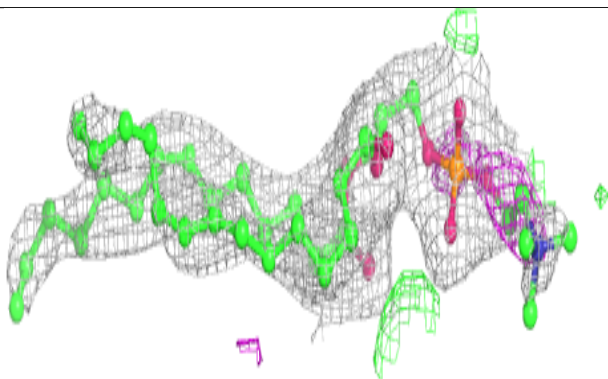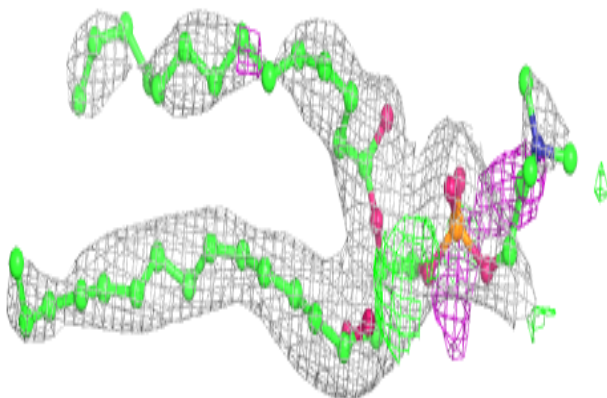
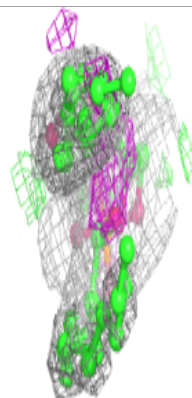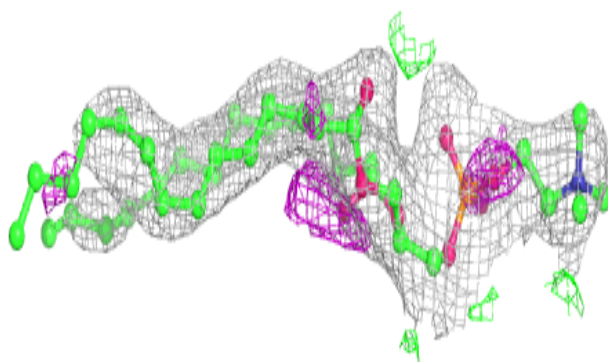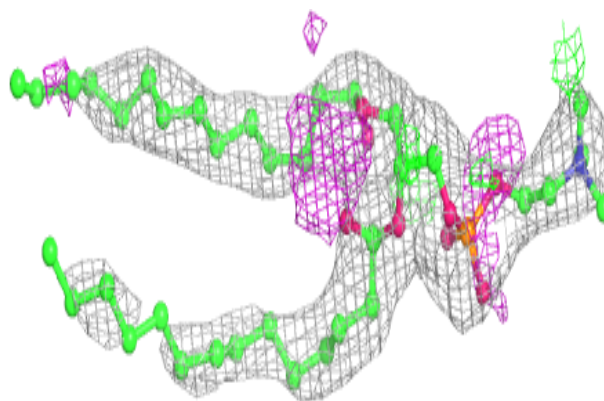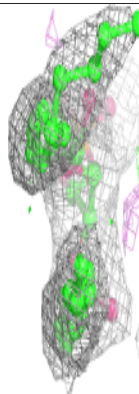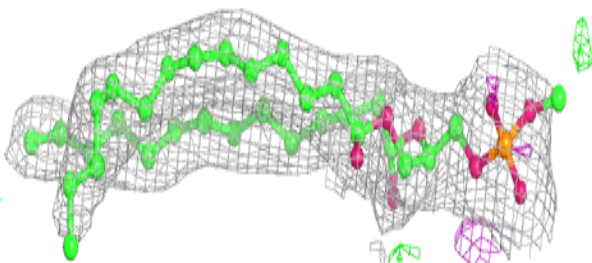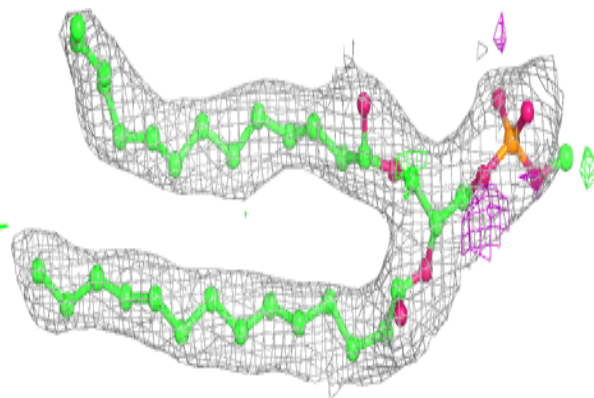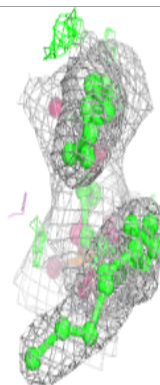**Electron density around CPS A 1304:**

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and green (positive)
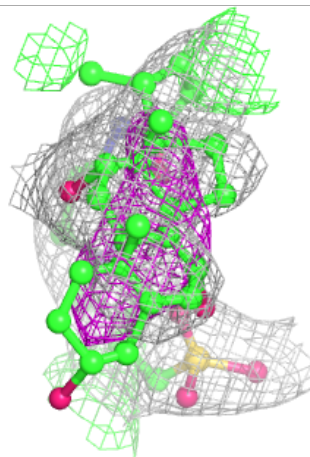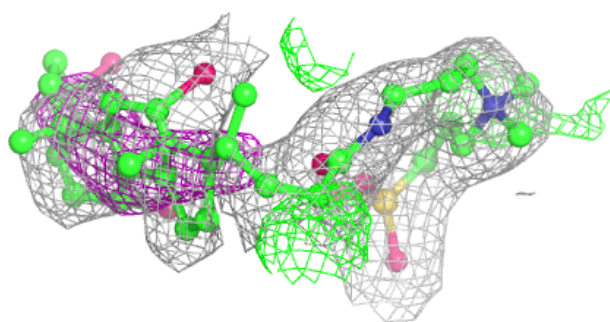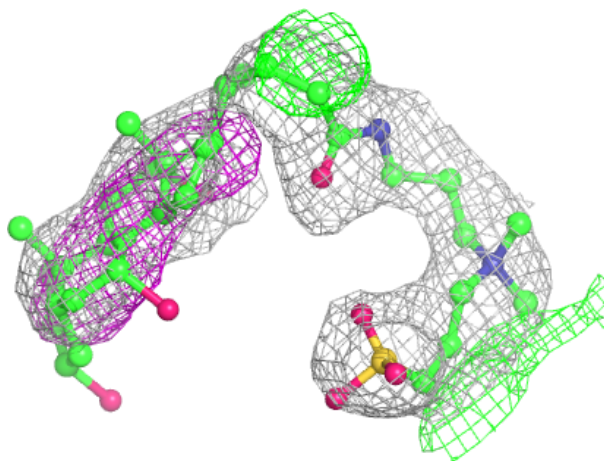
Electron density around CPS B 1308:

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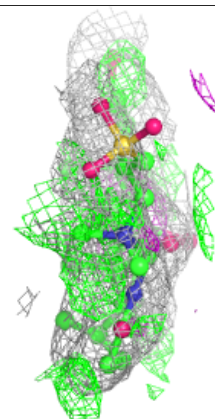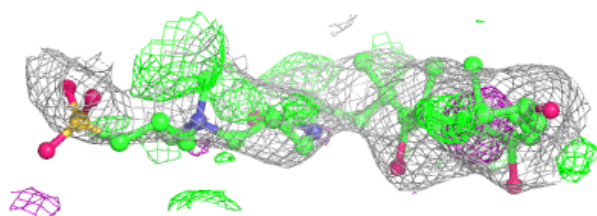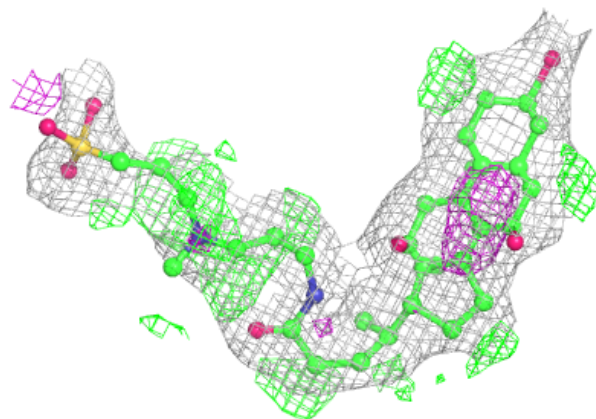
Electron density around MC3 D 1302:

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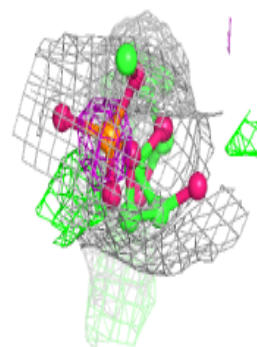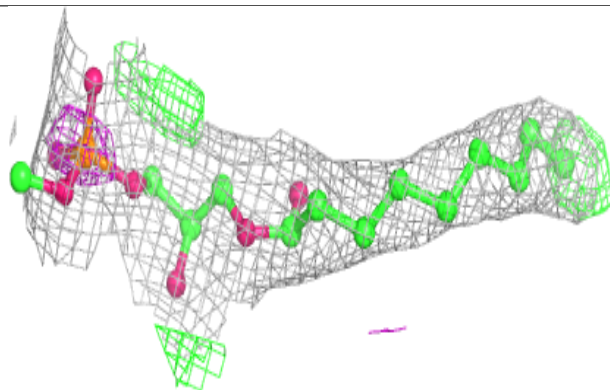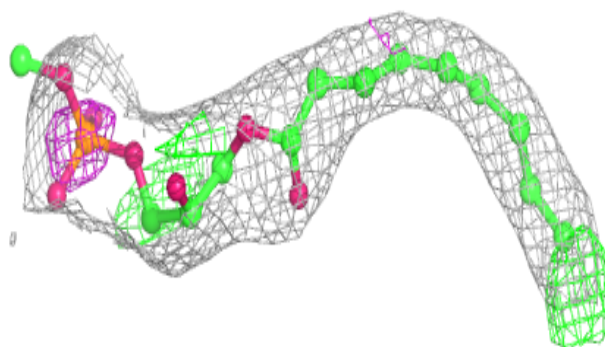
Electron density around CPS A 1306:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
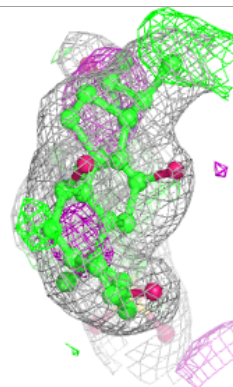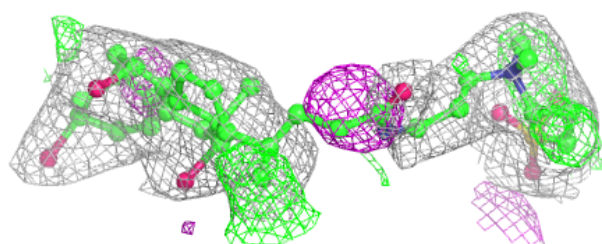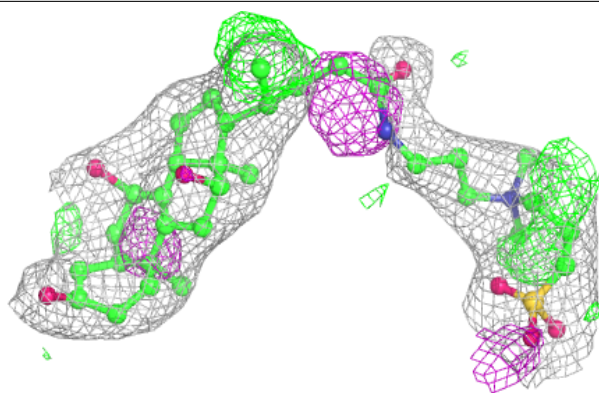
Electron density around CPS A 1305:

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and green (positive)
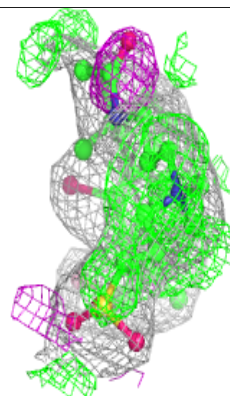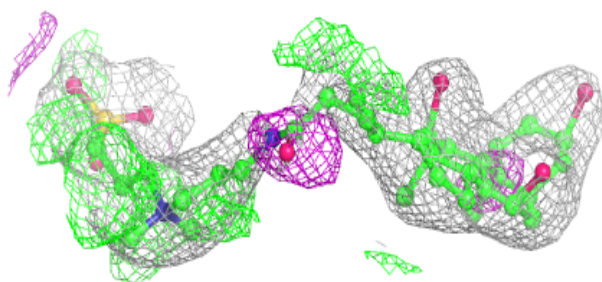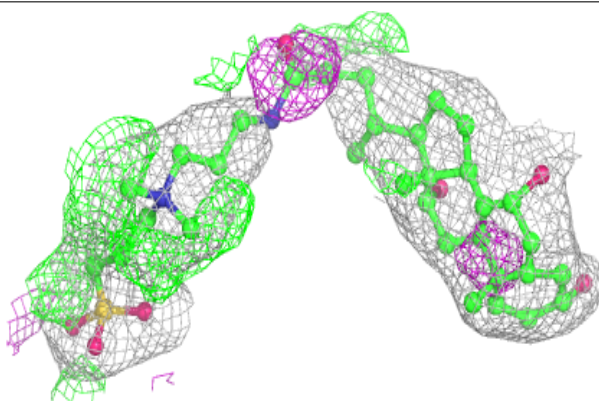
Electron density around CPS D 1308:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
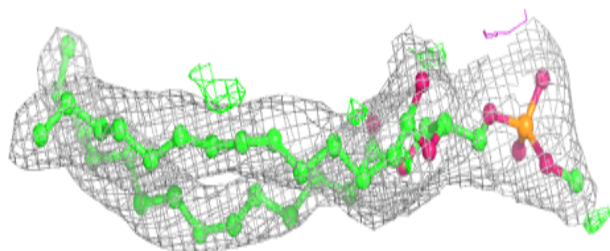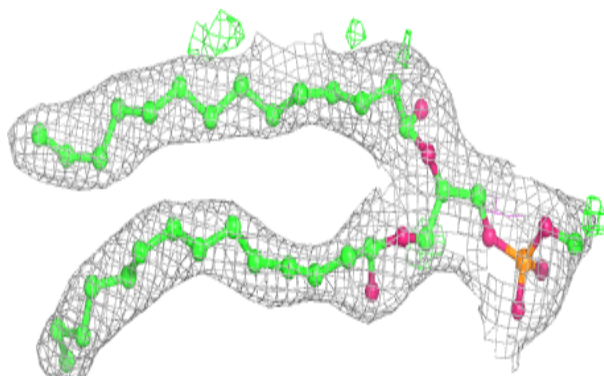mF_o-DF_c (at 3 rmsd) in purple (negative)
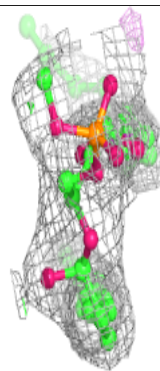and green (positive)
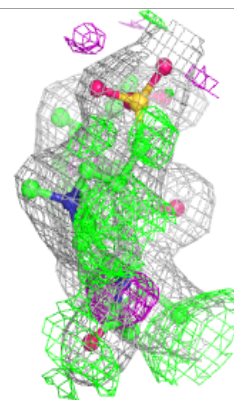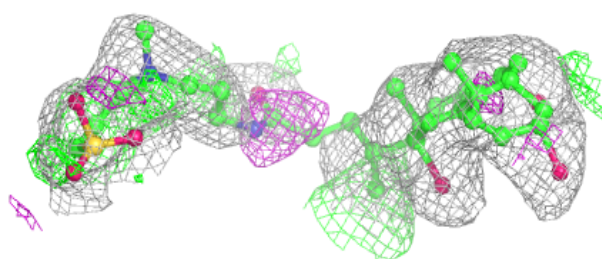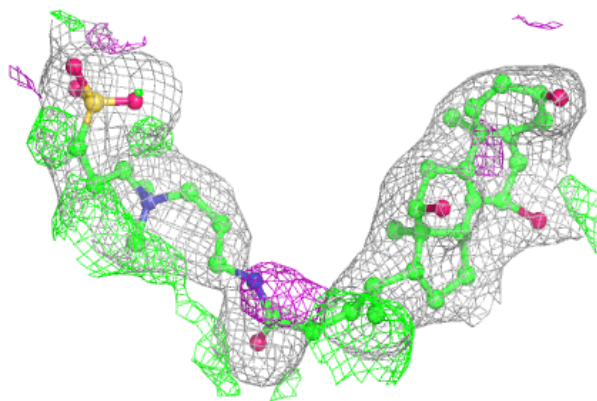
Electron density around MC3 C 1301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
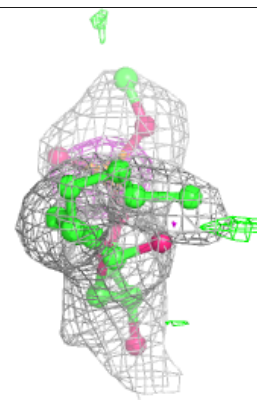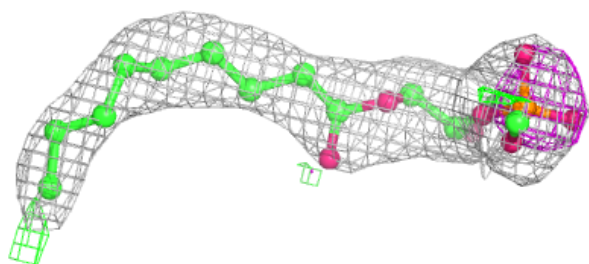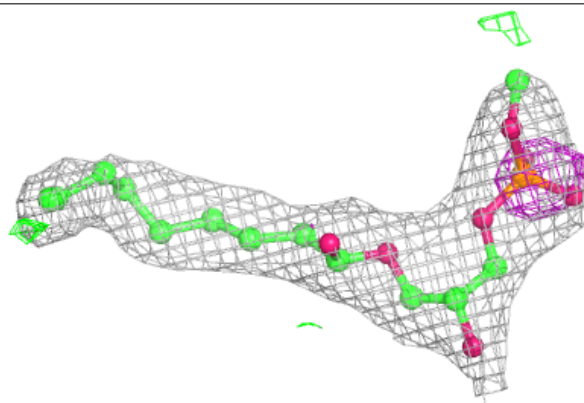
Electron density around MC3 B 1302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
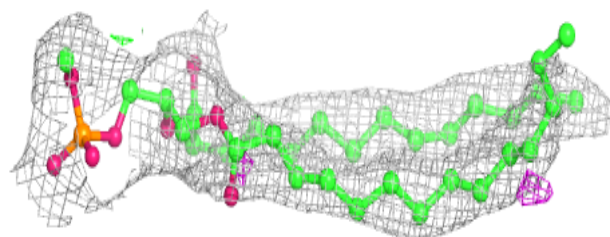mF_o-DF_c (at 3 rmsd) in purple (negative)
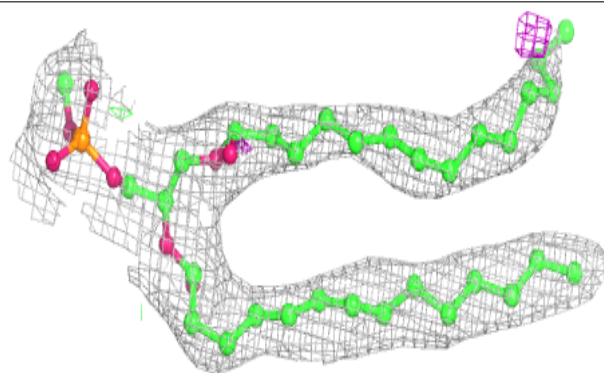and green (positive)
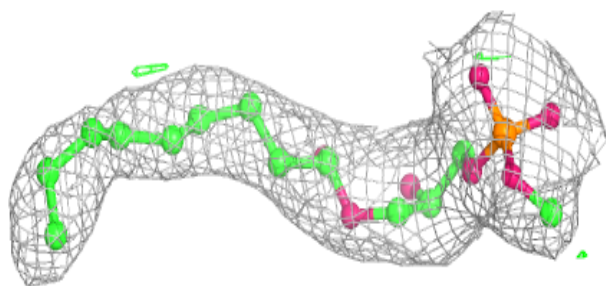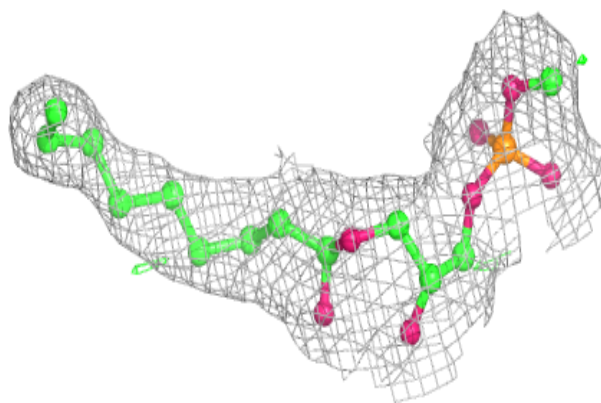
Electron density around MC3 A 1301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
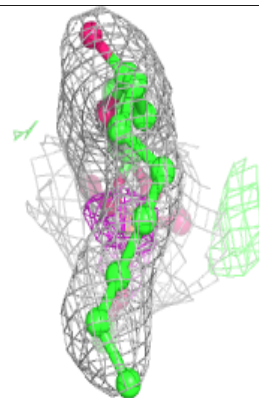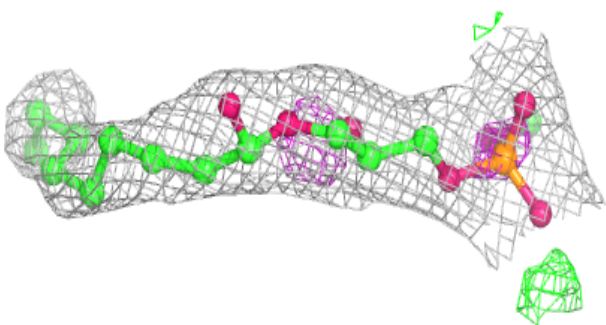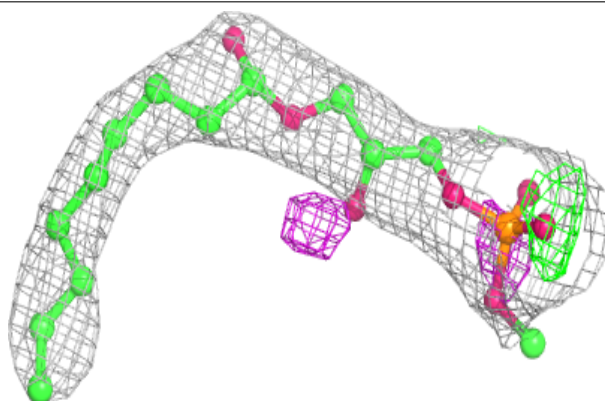
Electron density around MC3 C 1305:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
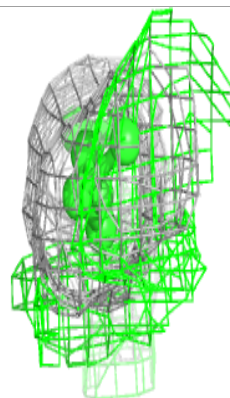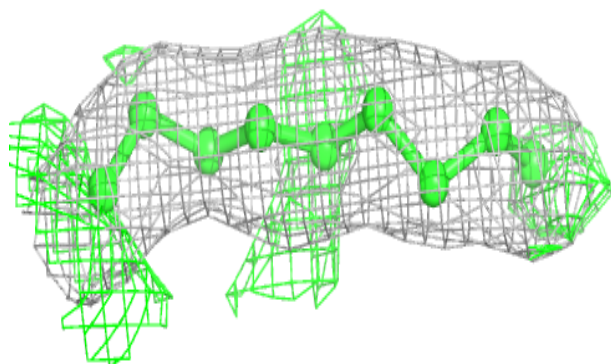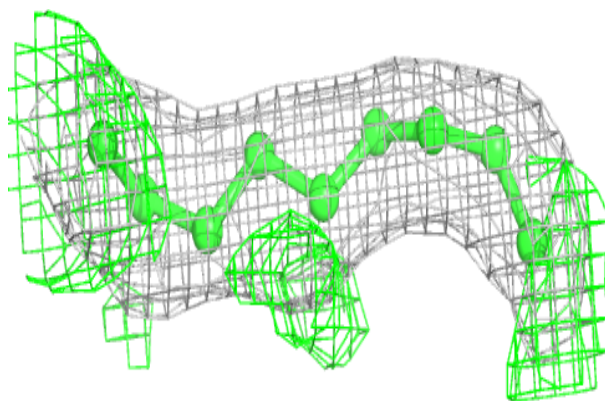
Electron density around CPS B 1307:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
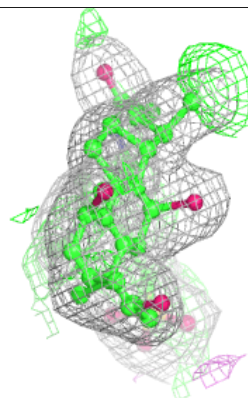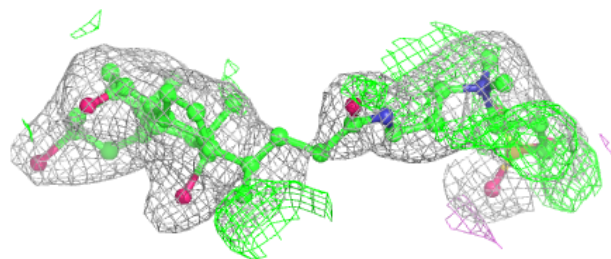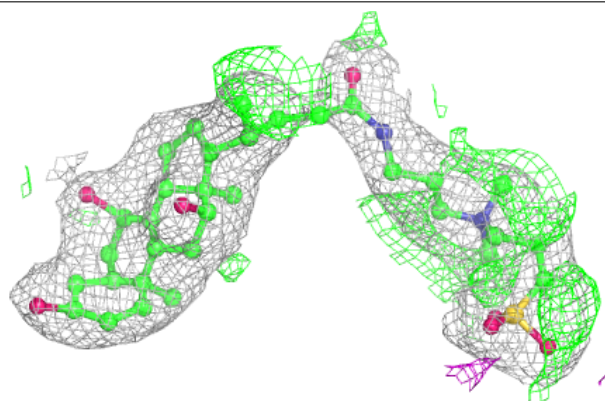
Electron density around MC3 B 1306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
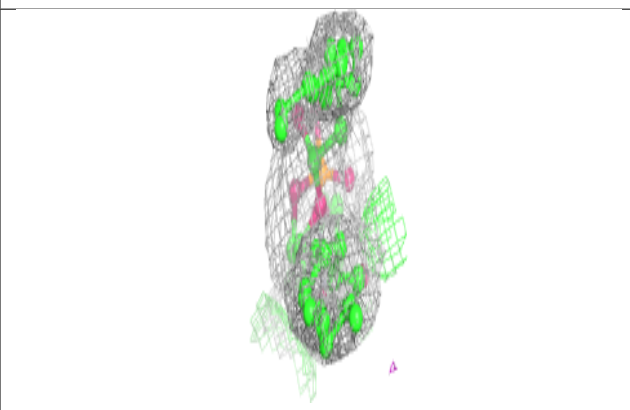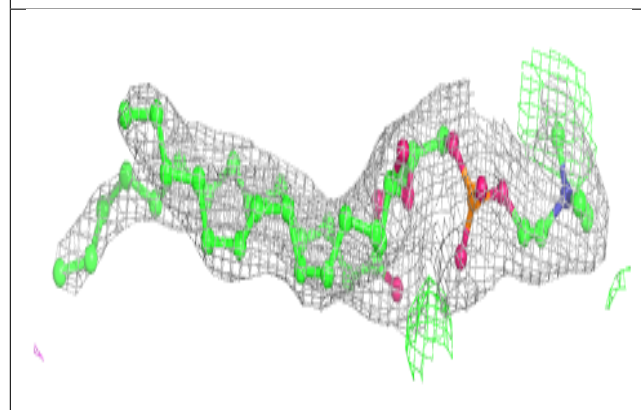mF_o-DF_c (at 3 rmsd) in purple (negative)
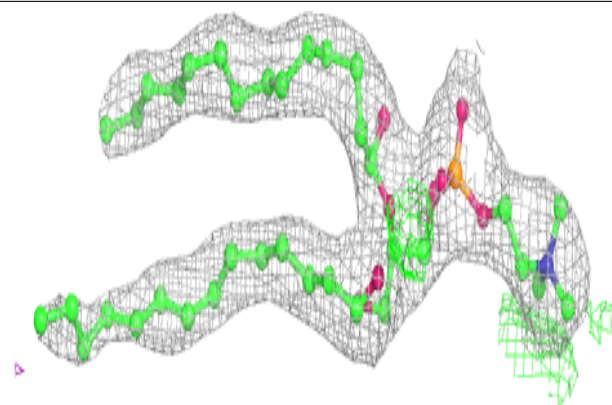and green (positive)
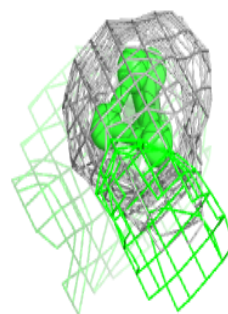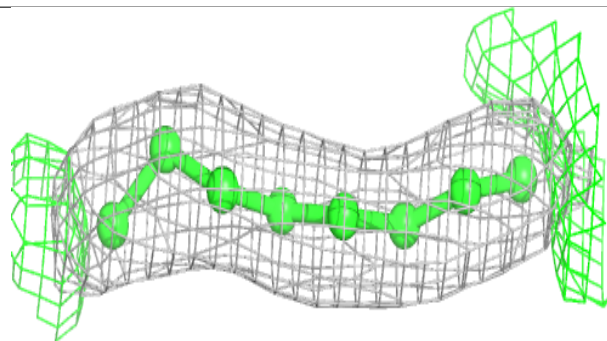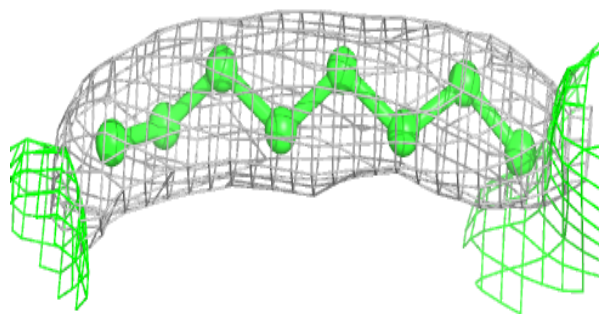
Electron density around MC3 C 1306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
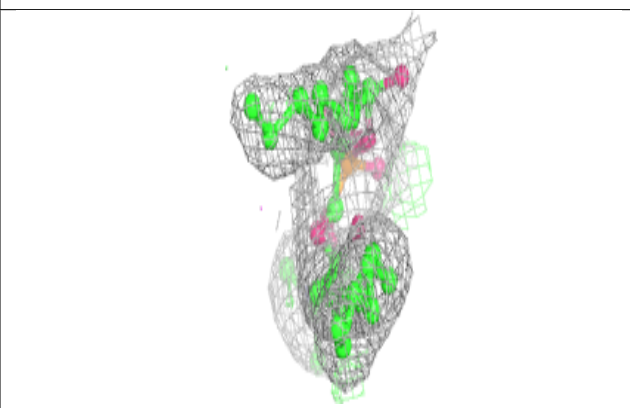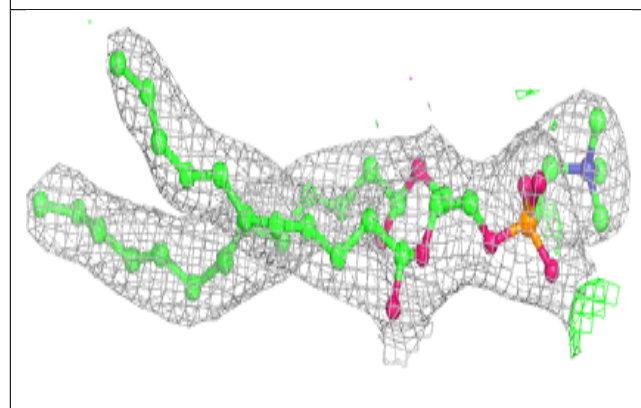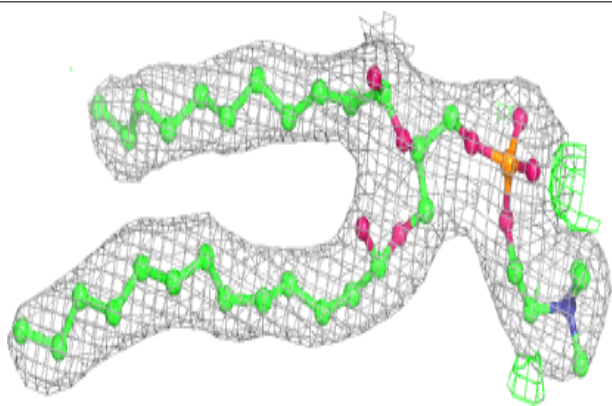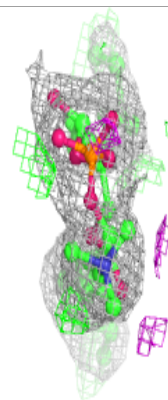and green (positive)
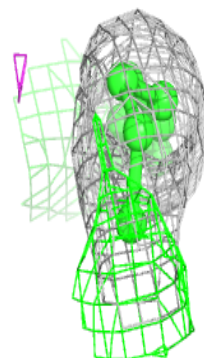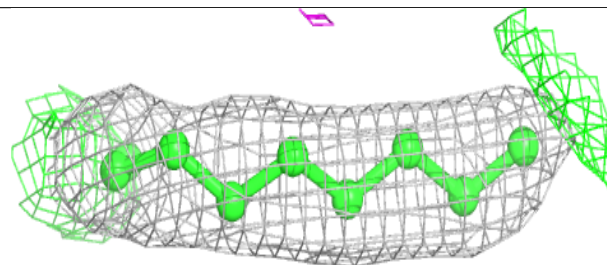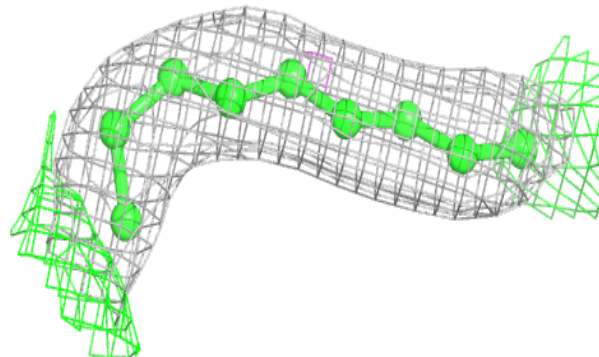
Electron density around MC3 C 1302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
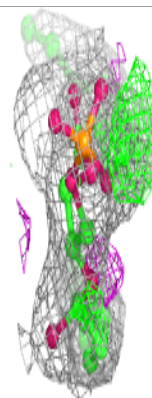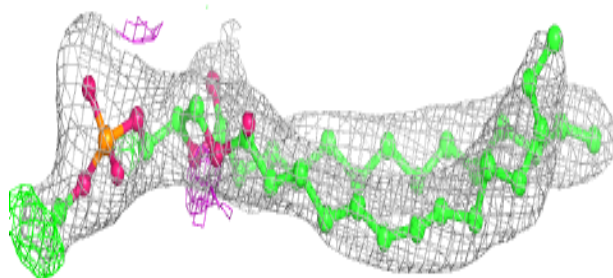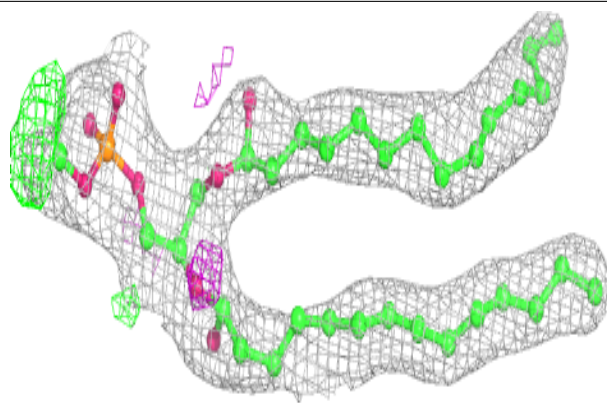
Electron density around MC3 C 1304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
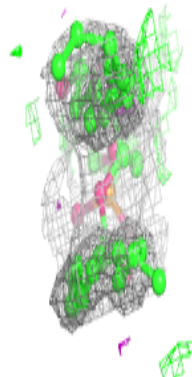
Electron density around MC3 D 1307:

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

Electron density around MC3 B 1305:

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

Electron density around MC3 A 1303:

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

Electron density around MC3 D 1303:

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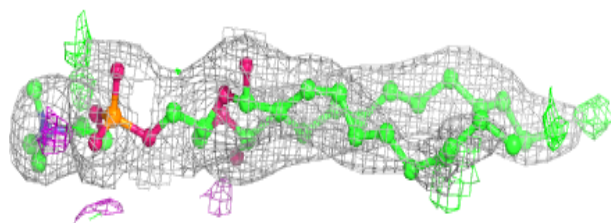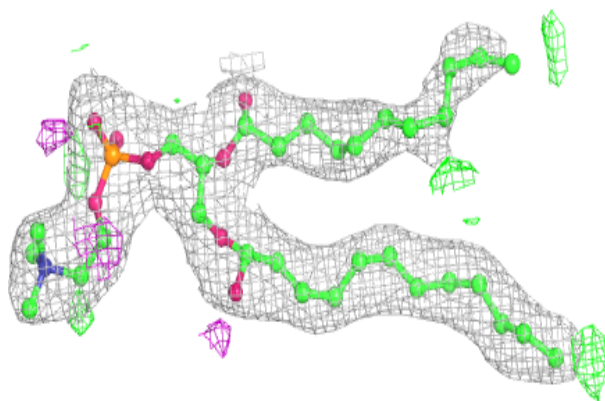$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around MC3 B 1303:

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

Electron density around MC3 C 1307:

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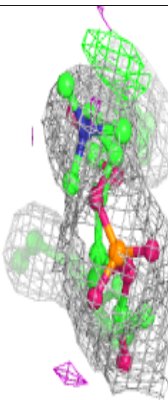mF_o-DF_c (at 3 rmsd) in purple (negative)
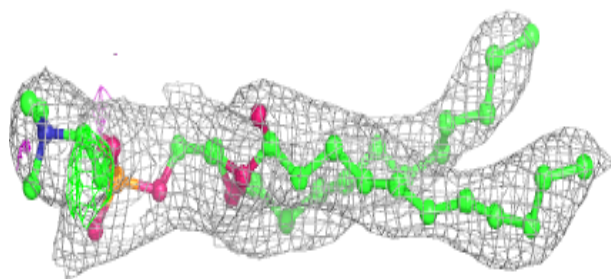and green (positive)

Electron density around MC3 D 1306:

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

Electron density around MC3 D 1305:

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

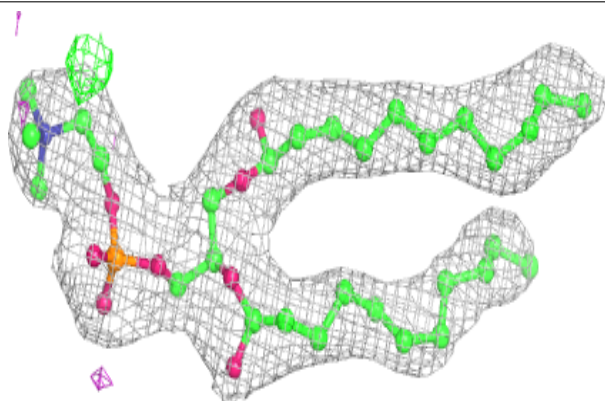**Electron density around MC3 B 1304:**

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 MC3 C 1303:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
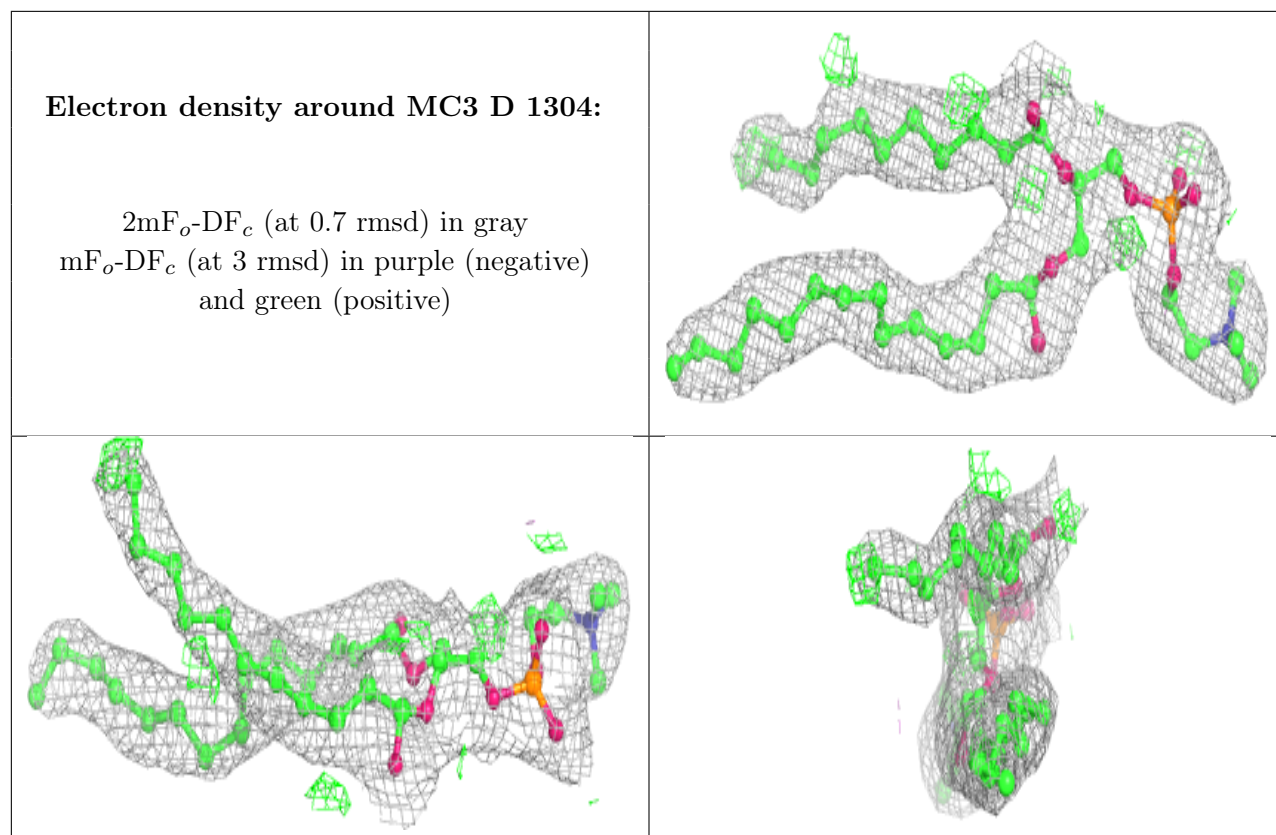mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around MC3 D 1304:

$2mF_o$-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.