WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 14, 2023 – 11:37 AM EDT

PDB ID	:	8E1U
Title	:	Propionibacterium freudenreichii PPi-dependent PEPCK in complex with malate
Authors	:	McLeod, M.J.; Holyoak, T.
Deposited on	:	2022-08-11
Resolution	:	2.65 Å(reported)

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

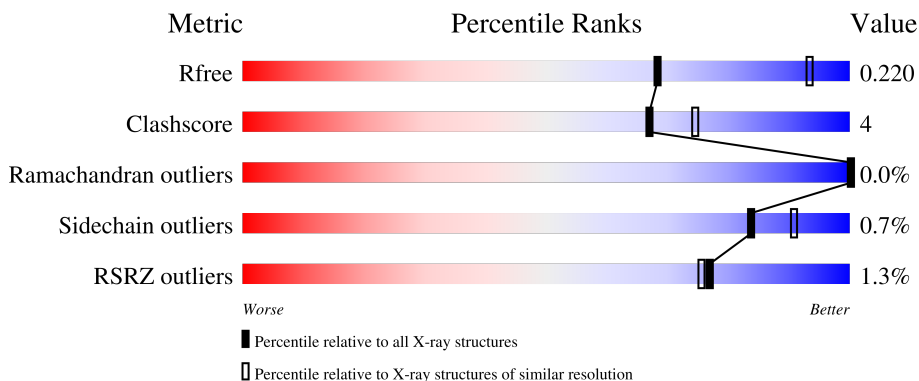|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.65 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		0.220
Clashscore		4
Ramachandran outliers		0.0%
Sidechain outliers		0.7%
RSRZ outliers		1.3%

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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	1131	89% 11%
1	B	1131	5% / 88% 11% •
1	C	1131	% / 90% 10% •
1	D	1131	% / 88% 11% •
1	E	1131	% / 88% 11% •

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Mol	Chain	Length	Quality of chain
1	F	1131	88% 10%
1	G	1131	87% 12%
1	H	1131	88% 11%

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	MLT	C	1202	-	-	-	X

2   Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 72470 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 PPi-dependent PEPCK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1126	Total 8928	C 5615	N 1574	O 1706	S 33	0	0	0
1	B	1125	Total 8921	C 5612	N 1573	O 1704	S 32	0	0	0
1	C	1125	Total 8922	C 5612	N 1573	O 1704	S 33	0	0	0
1	D	1124	Total 8914	C 5608	N 1572	O 1701	S 33	0	0	0
1	E	1120	Total 8881	C 5589	N 1567	O 1693	S 32	0	0	0
1	F	1117	Total 8868	C 5581	N 1564	O 1690	S 33	0	0	0
1	G	1115	Total 8859	C 5576	N 1562	O 1688	S 33	0	0	0
1	H	1122	Total 8895	C 5598	N 1567	O 1697	S 33	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0
2	E	1	Total 1	Mg 1	0	0
2	F	1	Total 1	Mg 1	0	0

W O R L D W I D E
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PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Mg 1	0	0
2	H	1	Total 1	Mg 1	0	0

- Molecule 3 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$) (labeled as "Ligand of Interest" by depositor).

MLT
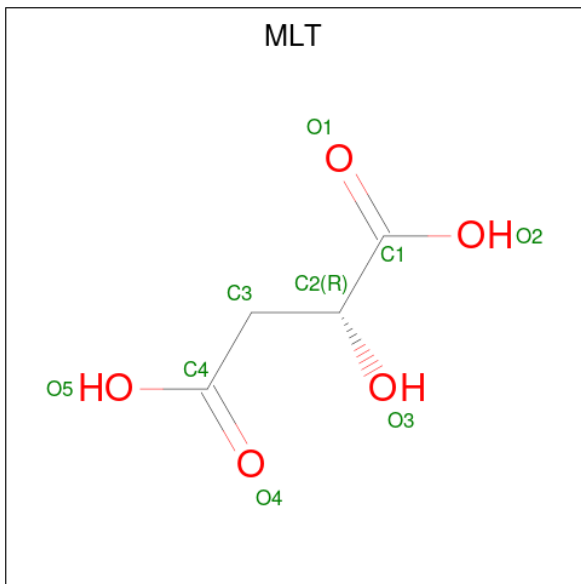
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 9	C 4	O 5	0	0
3	B	1	Total 9	C 4	O 5	0	0
3	C	1	Total 9	C 4	O 5	0	0
3	F	1	Total 9	C 4	O 5	0	0
3	G	1	Total 9	C 4	O 5	0	0
3	H	1	Total 9	C 4	O 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total 193	O 193	0	0

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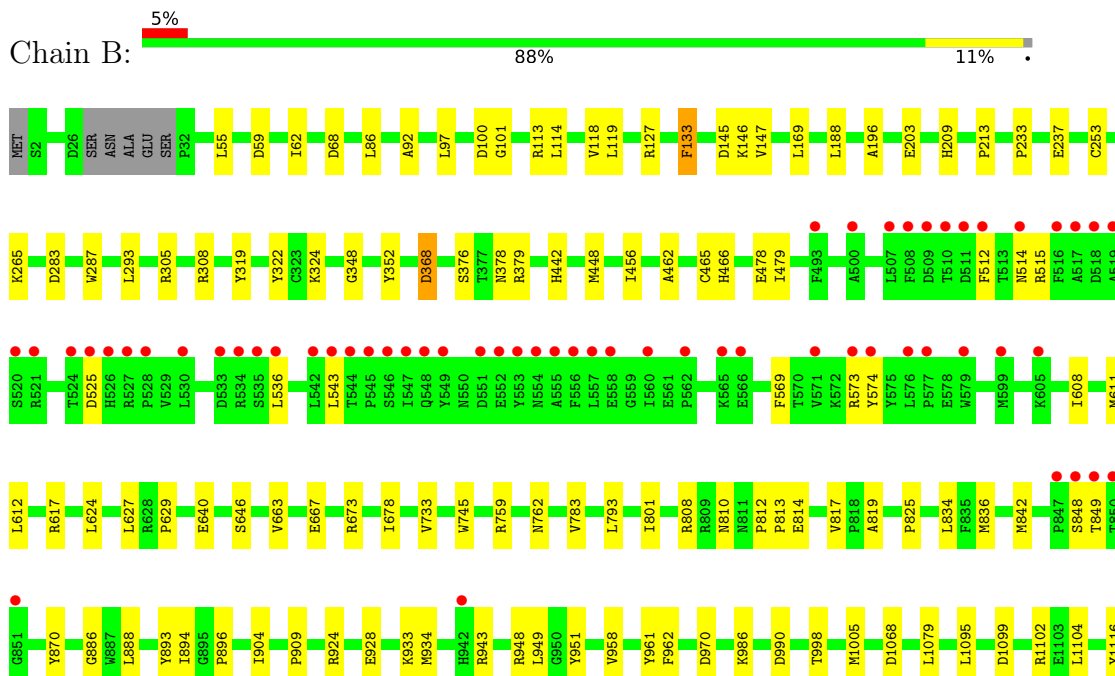| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	122	Total 122	O 122	0	0
4	C	141	Total 141	O 141	0	0
4	D	156	Total 156	O 156	0	0
4	E	144	Total 144	O 144	0	0
4	F	173	Total 173	O 173	0	0
4	G	137	Total 137	O 137	0	0
4	H	154	Total 154	O 154	0	0

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.
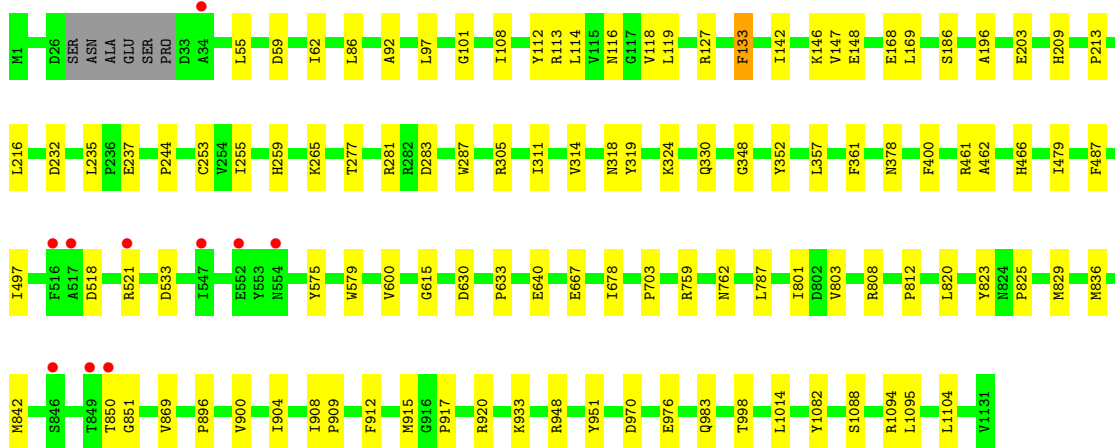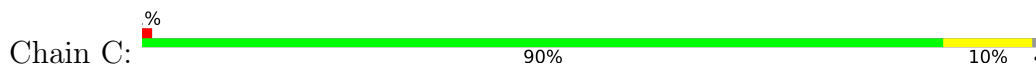
- Molecule 1: PPi-dependent PEPCK
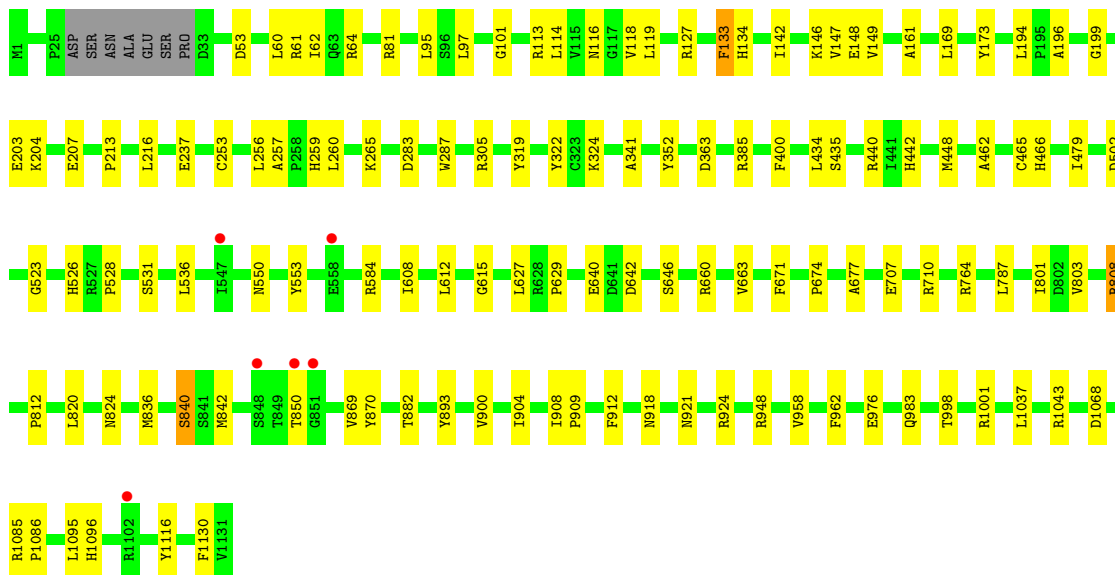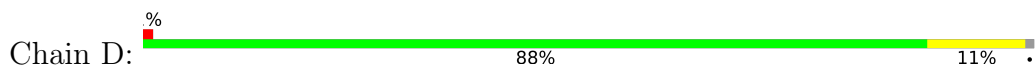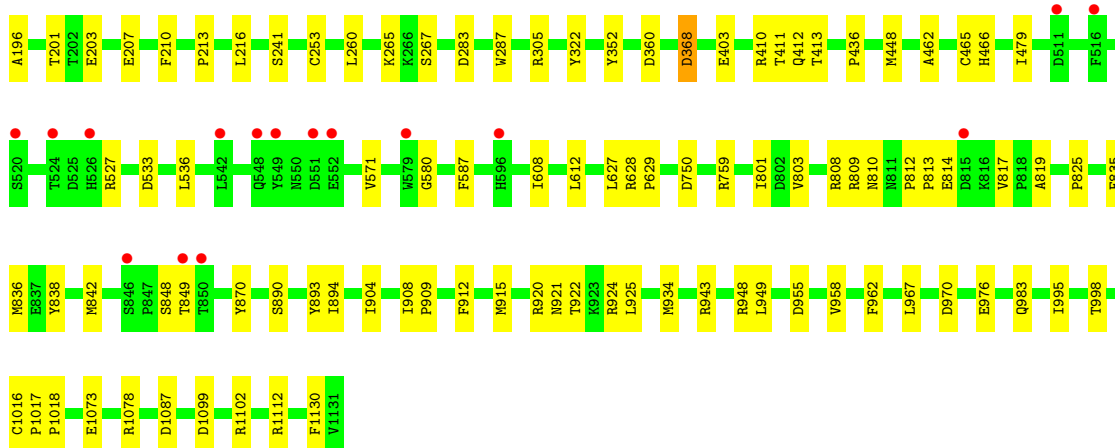

Chain A:

- Molecule 1: PPi-dependent PEPCK

Chain B:

R1129 F1130 V1131

● Molecule 1: PPi-dependent PEPCK

Chain C:

%

90%   10%

M1 D26 SER ASN ALA GLU SER PRO D33 A34 L55 D59 I62 L86 A92 L97 G101 I108 Y112 R113 L114 V115 N116 G117 V118 L119 R127 F133 I142 K146 V147 E148 E168 L169 S186 A196 E203 H209 P213

L216 D232 L235 P236 E237 P244 C253 V254 I255 H259 K265 T277 R281 R282 D283 W287 R305 I311 V314 N318 Y319 K324 Q330 G348 Y352 L357 F361 N378 F400 R461 A462 H466 I479 F487

I497 F516 A517 D518 R521 D533 T547 E552 Y553 N554 Y575 W579 V600 G615 D630 P633 E640 E667 I678 P703 R759 N762 L787 I801 D802 V803 R808 P812 L820 Y823 N824 P825 M829 M836

M842 S846 T849 T850 G851 V869 P896 V900 I904 I908 P909 F912 M915 G916 P917 R920 K933 R948 Y951 D970 E976 Q983 T998 L1014 Y1082 S1088 R1094 L1095 L1104 V1131

● Molecule 1: PPi-dependent PEPCK

Chain D:

%

88%   11%

M1 P25 ASP SER ASN ALA GLU SER PRO D33 D53 L60 R61 I62 Q63 R64 R81 L95 S96 L97 G101 R113 L114 V115 N116 G117 V118 L119 R127 F133 H134 I142 K146 V147 E148 V149 A161 L169 Y173 L194 P195 A196 G199

E203 K204 E207 P213 L216 E237 C253 L256 A257 P258 H259 L260 K265 D283 W287 R305 Y319 Y322 C323 K324 A341 Y352 D363 R385 F400 L434 S435 R440 I441 H442 M448 A462 C465 H466 I479 D502

G523 H526 R527 P528 S531 L536 T547 N550 Y553 E558 R584 I608 L612 G615 L627 R628 P629 E640 D641 D642 S646 R660 V663 F671 P674 A677 E707 R710 R764 L787 I801 D802 V803 R808

P812 L820 N824 M836 S840 S841 M842 S848 T849 T850 G851 V869 Y870 T882 Y893 V900 I904 I908 P909 F912 N918 N921 R924 R948 V958 F962 E976 Q983 T998 R1001 L1037 R1043 D1068

R1085 P1086 L1095 H1096 R1102 Y1116 F1130 V1131

● Molecule 1: PPi-dependent PEPCK

Chain E:

%

88%   11%

MET S2 P25 ASP SER ASN ALA GLU SER PRO ASP A34 I35 L51 LYS ASP R54 R61 I62 D72 L97 D100 G101 F104 S111 Y112 R113 L114 V115 N116 G117 V118 L119 R127 F133 K146 V147 R160 A161 D166 L169 S186 L194 P195

A196 T201 T202 E203 E207 F210 P213 L216 S241 C253 L260 K265 K266 S267 D283 W287 R305 Y322 Y352 D360 D368 E403 R410 T411 Q412 T413 P436 M448 A462 C465 H466 I479 D511 F516

S520 T524 D525 H526 R527 D533 L536 L542 Q548 Y549 N550 D551 E552 V571 W579 G580 F587 H596 I608 L612 L627 R628 P629 D750 R759 I801 D802 V803 R808 R809 N810 N811 P812 P813 E814 D815 K816 V817 P818 A819 P825 F835

M836 E837 Y838 M842 S846 P847 S848 T849 T850 Y870 S890 Y893 I894 I904 I908 P909 F912 M915 R920 N921 T922 K923 R924 L925 M934 R943 R948 L949 D955 V958 F962 L967 D970 E976 Q983 I995 T998

C1016 P1017 P1018 E1073 R1078 D1087 D1099 R1102 R1112 F1130 V1131

● Molecule 1: PPi-dependent PEPCK

Chain F:

88%   10%   ·

M1 S2 V3 R7 P25 ASP SER ASN ALA GLU SER PRO D33 A34 I35 S48 L51 K52 D53 R54 L55 D59 L60 R61 I62 D72 R81 L97 D100 I108 Y112 R113 L114 V115 N116 G117 V118 L119 R127 F133 H134 L140 D145 K146 V147

E148 V149 Y154 L169 L194 P195 A196 E203 E207 P213 L216 P244 C253 A257 P258 H259 K265 M270 D283 G284 Q285 C286 W287 N295 F300 K301 V302 R305 D306 N318 Y319 Y322 C323 K324 A341 E344 Y352 E387

H454 L455 I456 A462 H466 I479 F516 R527 R534 S535 L536 N550 F569 K605 L612 G615 F616 R617 R623 L627 R628 P629 D642 S646 K661 Y662 V663 D695 P703 D756 I801 R808 P812 P813 K816

A819 L820 P825 L831 M836 M842 T843 G844 LYS SER PRO SER THR THR GLY A852 Y879 Y893 P896 V900 I904 P909 K923 R924 E928 R948 D955 L967 D970 K986 D990 T998 R1020 D1038 E1073 L1079

D1099 R1102 E1103 L1104 R1112 V1131

● Molecule 1: PPi-dependent PEPCK

Chain G:

%

87%   12%   ·

M1 P25 ASP SER ASN ALA GLU SER PRO D33 A34 E46 R49 D59 L60 R61 D72 L95 S96 L97 D100 G101 Y112 R113 L114 V115 N116 G117 V118 L119 R127 F133 L140 Q144 D145 K146 V147 R160 L169 Y173 S186 A196

E203 E207 V208 H209 F210 P213 L216 P244 L256 K265 K266 S267 D274 D283 W287 L293 R305 D306 Y322 G340 Y352 P353 D368 N378 L382 F400 Q452 S459 A462 C465 H466 I479 F493 D502

L507 P528 V529 L530 S531 I532 L536 G537 K541 L542 L543 N554 E558 G559 I560 Y574 G580 R584 G590 R595 N598 R601 K605 G615 R628 P629 D630 S646 T647 V648 V663 P703 V733 W745 L787 I801 R808

P813 E814 D815 K816 V817 P818 A819 Y823 N824 P825 M836 M842 T843 GLY LYS SER PRO SER THR GLY ALA G853 Y870 S878 T882 L888 I894 A898 R899 V900 I904 I908 P909 H914 K933 M934 R948 L949 G950 Y951 V958 F962

G963 R964 L967 D970 R979 L982 K986 D990 T998 R1001 D1009 E1024 S1031 D1099 R1102 E1103 L1104 T1123 L1124 G1125 R1129 F1130 V1131

• Molecule 1: PPi-dependent PEPCK

Chain H:

%

88%   11%   •

M1 L20 P25 ASP SER ASN ALA GLU SER P32 R49 D53 R54 L55 D59 I62 D72 C73 D74 R81 L97 D100 G101 D102 R113 L114 V118 L119 R127 F133 V147 R156 A161 E168 L169 S186 V193 A196

E203 E207 F210 P213 L216 D232 L235 P244 T251 G252 C253 A257 P258 H259 L260 K265 D283 W287 R305 V310 Y322 C323 K324 I331 Y352 N358 Q359 D360 D368 R410 A418 Q423 H445 R446 W453 H454

L455 I456 A462 C465 H466 I479 F493 I540 N554 E558 F569 R573 I591 K605 L612 G615 F616 R617 L627 R628 P629 D642 S646 V663 P674 D675 D676 A677 A691 L729 V733 W745 V783 L793 I801

R808 R809 N810 N811 P812 P813 A819 P825 L834 M842 S846 P847 S848 T849 T850 Y870 G886 Y893 I894 V900 I904 P909 N918 R924 M934 D940 G941 H942 L949 D955 V958 F962 E976 Q983 K986 D990

T998 R1001 R1020 A1021 L1022 M1026 L1079 E1084 ARG PRO ASP S1088 L1095 L1104 F1130 V1131

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	134.13Å 146.95Å 151.09Å 82.70° 84.00° 70.80°	Depositor
Resolution (Å)	74.77 – 2.65 74.77 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.0 (74.77-2.65) 96.9 (74.77-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, REFMAC 8.0.006	Depositor
R, R_{free}	0.181 , 0.223 0.181 , 0.220	Depositor DCC
R_{free} test set	2000 reflections (0.66%)	wwPDB-VP
Wilson B-factor (Å^2)	45.2	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.5	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	72470	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: MG, MLT

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	0.25	0/9149	0.49	0/12433
1	B	0.24	0/9143	0.49	0/12426
1	C	0.25	0/9143	0.49	0/12425
1	D	0.25	0/9135	0.49	0/12414
1	E	0.25	0/9101	0.49	0/12368
1	F	0.25	0/9087	0.49	0/12347
1	G	0.25	0/9078	0.49	0/12335
1	H	0.25	0/9115	0.49	0/12385
All	All	0.25	0/72951	0.49	0/99133

There are no bond length outliers.

There are no bond angle outliers.

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	8928	0	8656	69	0
1	B	8921	0	8647	68	0
1	C	8922	0	8651	61	0
1	D	8914	0	8647	68	0
1	E	8881	0	8613	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	8868	0	8599	70	0
1	G	8859	0	8591	80	0
1	H	8895	0	8630	69	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	9	0	4	0	0
3	B	9	0	4	0	0
3	C	9	0	4	0	0
3	F	9	0	4	0	0
3	G	9	0	4	0	0
3	H	9	0	4	1	0
4	A	193	0	0	1	0
4	B	122	0	0	0	0
4	C	141	0	0	0	0
4	D	156	0	0	1	0
4	E	144	0	0	2	0
4	F	173	0	0	0	0
4	G	137	0	0	1	0
4	H	154	0	0	1	0
All	All	72470	0	69058	547	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 547 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:F:53:ASP:HA	1:F:81:ARG:HB3	1.67	0.76
1:H:53:ASP:HA	1:H:81:ARG:HB3	1.69	0.74
1:B:169:LEU:HD23	1:B:213:PRO:HB3	1.71	0.72
1:A:53:ASP:HA	1:A:81:ARG:HB3	1.70	0.72
1:D:479:ILE:HG13	1:D:909:PRO:HG3	1.72	0.71

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	1122/1131 (99%)	1094 (98%)	28 (2%)	0	100	100
1	B	1121/1131 (99%)	1075 (96%)	46 (4%)	0	100	100
1	C	1121/1131 (99%)	1090 (97%)	31 (3%)	0	100	100
1	D	1120/1131 (99%)	1084 (97%)	36 (3%)	0	100	100
1	E	1114/1131 (98%)	1084 (97%)	29 (3%)	1 (0%)	51	69
1	F	1111/1131 (98%)	1073 (97%)	38 (3%)	0	100	100
1	G	1109/1131 (98%)	1075 (97%)	34 (3%)	0	100	100
1	H	1116/1131 (99%)	1086 (97%)	29 (3%)	1 (0%)	51	69
All	All	8934/9048 (99%)	8661 (97%)	271 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	849	THR
1	E	580	GLY

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	964/968 (100%)	953 (99%)	11 (1%)	73	85
1	B	963/968 (100%)	956 (99%)	7 (1%)	84	91
1	C	963/968 (100%)	959 (100%)	4 (0%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	962/968 (99%)	955 (99%)	7 (1%)	84	91
1	E	958/968 (99%)	952 (99%)	6 (1%)	86	92
1	F	956/968 (99%)	951 (100%)	5 (0%)	88	94
1	G	956/968 (99%)	951 (100%)	5 (0%)	88	94
1	H	960/968 (99%)	948 (99%)	12 (1%)	69	82
All	All	7682/7744 (99%)	7625 (99%)	57 (1%)	84	91

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	869	VAL
1	H	1020	ARG
1	F	54	ARG
1	H	940	ASP
1	H	368	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	717	GLN

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 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	#$|Z| > 2$
3	MLT	B	1202	-	8,8,8	1.04	0	10,10,10	1.54	2 (20%)
3	MLT	A	1202	-	8,8,8	1.03	0	10,10,10	1.62	2 (20%)
3	MLT	F	1202	-	8,8,8	1.04	0	10,10,10	1.56	2 (20%)
3	MLT	G	1202	-	8,8,8	1.03	0	10,10,10	1.69	2 (20%)
3	MLT	H	1202	-	8,8,8	1.04	0	10,10,10	1.66	1 (10%)
3	MLT	C	1202	-	8,8,8	1.03	0	10,10,10	1.58	1 (10%)

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
3	MLT	B	1202	-	-	5/8/8/8	-
3	MLT	A	1202	-	-	6/8/8/8	-
3	MLT	F	1202	-	-	4/8/8/8	-
3	MLT	G	1202	-	-	3/8/8/8	-
3	MLT	H	1202	-	-	5/8/8/8	-
3	MLT	C	1202	-	-	6/8/8/8	-

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1202	MLT	O2-C1-C2	3.65	120.73	112.72
3	G	1202	MLT	O2-C1-C2	3.60	120.62	112.72
3	C	1202	MLT	O2-C1-C2	3.48	120.36	112.72
3	A	1202	MLT	O2-C1-C2	3.32	120.01	112.72
3	F	1202	MLT	O2-C1-C2	3.17	119.69	112.72

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1202	MLT	O3-C2-C3-C4
3	C	1202	MLT	O1-C1-C2-O3
3	C	1202	MLT	O2-C1-C2-O3
3	F	1202	MLT	O1-C1-C2-O3
3	F	1202	MLT	O2-C1-C2-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1202	MLT	1	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 MLT B 1202

Bond lengths

Bond angles

Torsions

Rings

Ligand MLT A 1202

Bond lengths

Bond angles

Torsions

Rings

Ligand MLT F 1202

Bond lengths

Bond angles

Torsions

Rings

Ligand MLT G 1202

Bond lengths

Bond angles

Torsions

Rings

Ligand MLT H 1202

Bond lengths

Bond angles

Torsions

Rings

Ligand MLT C 1202

Bond lengths

Bond angles

Torsions

Rings
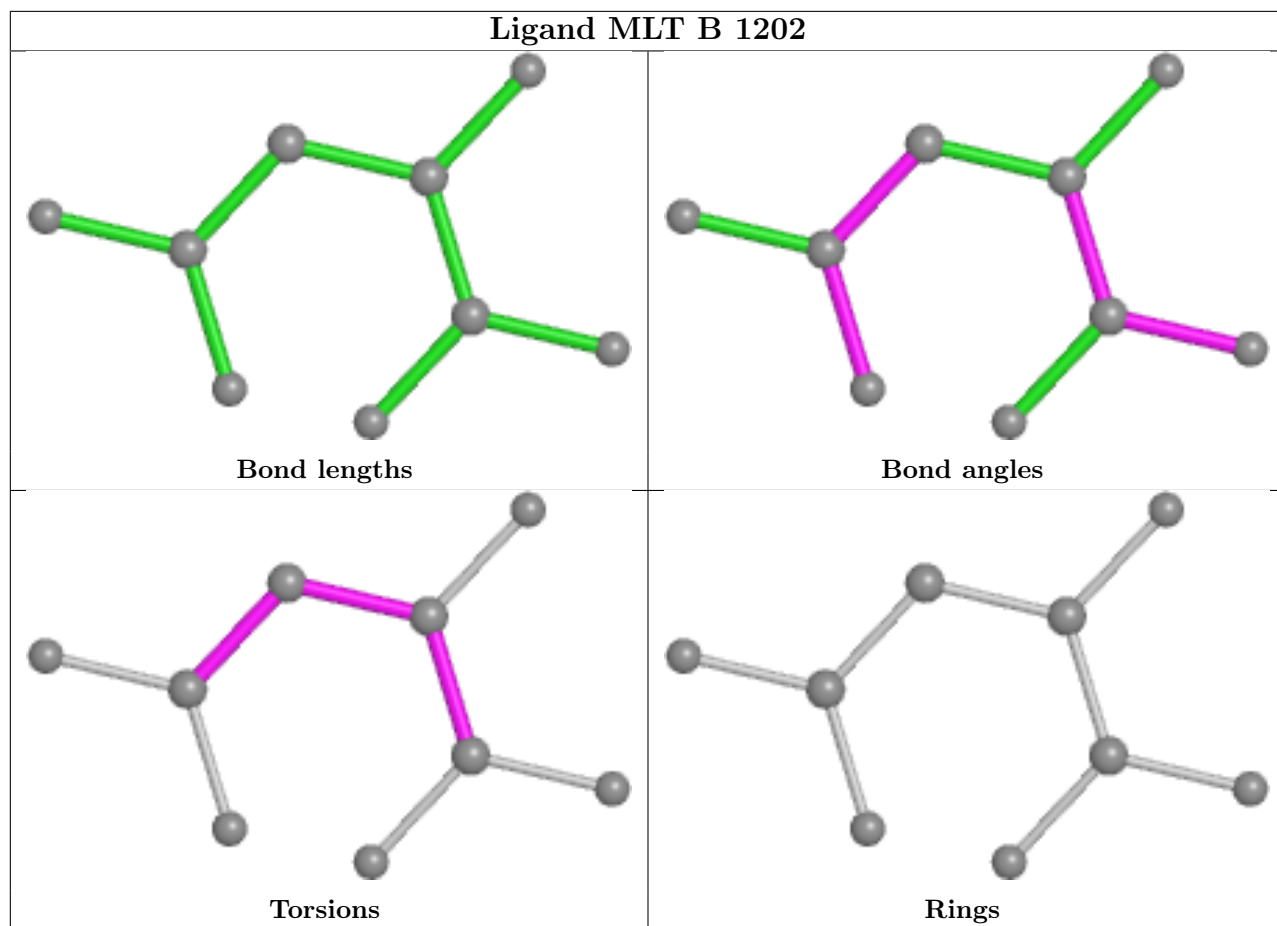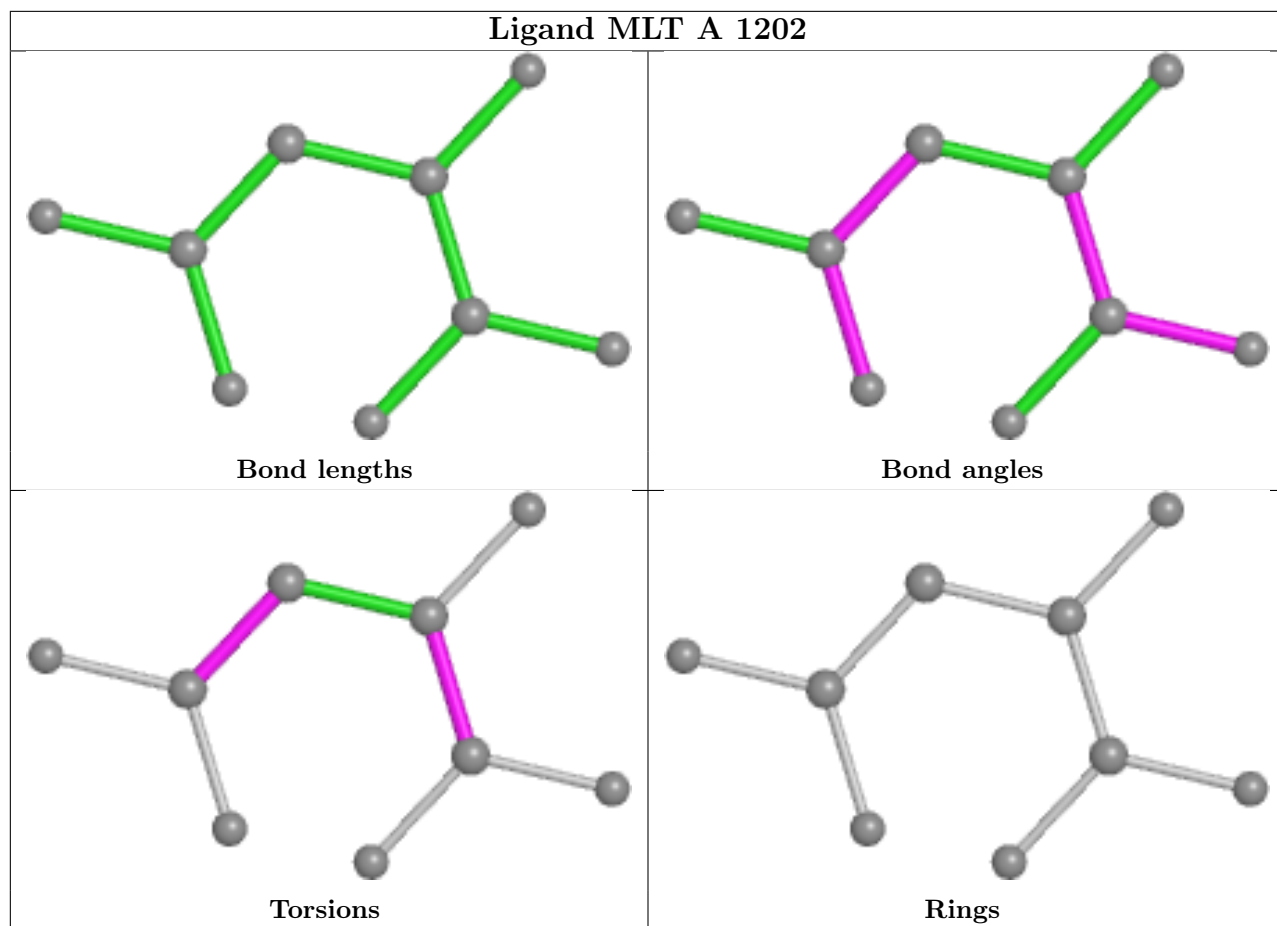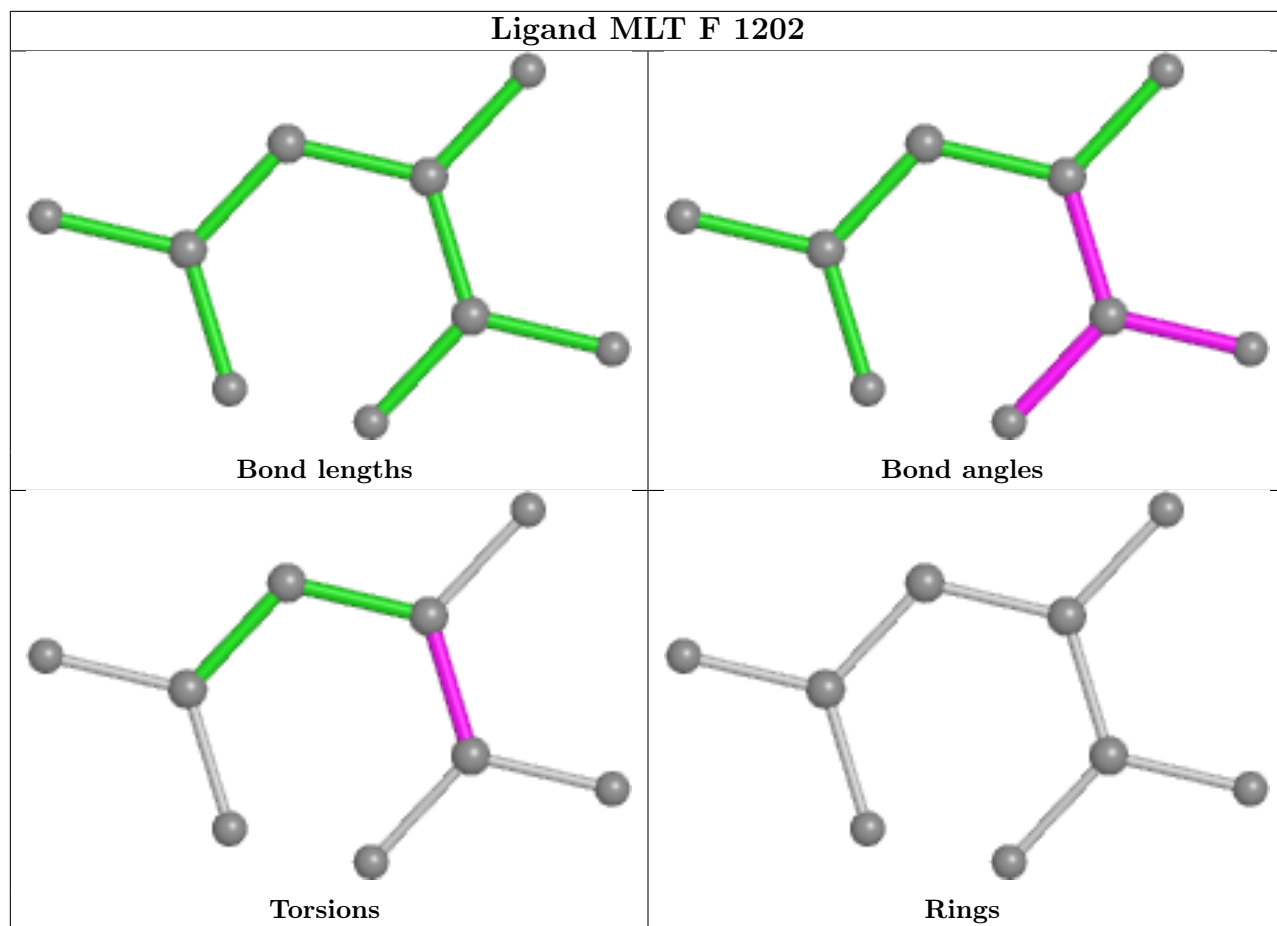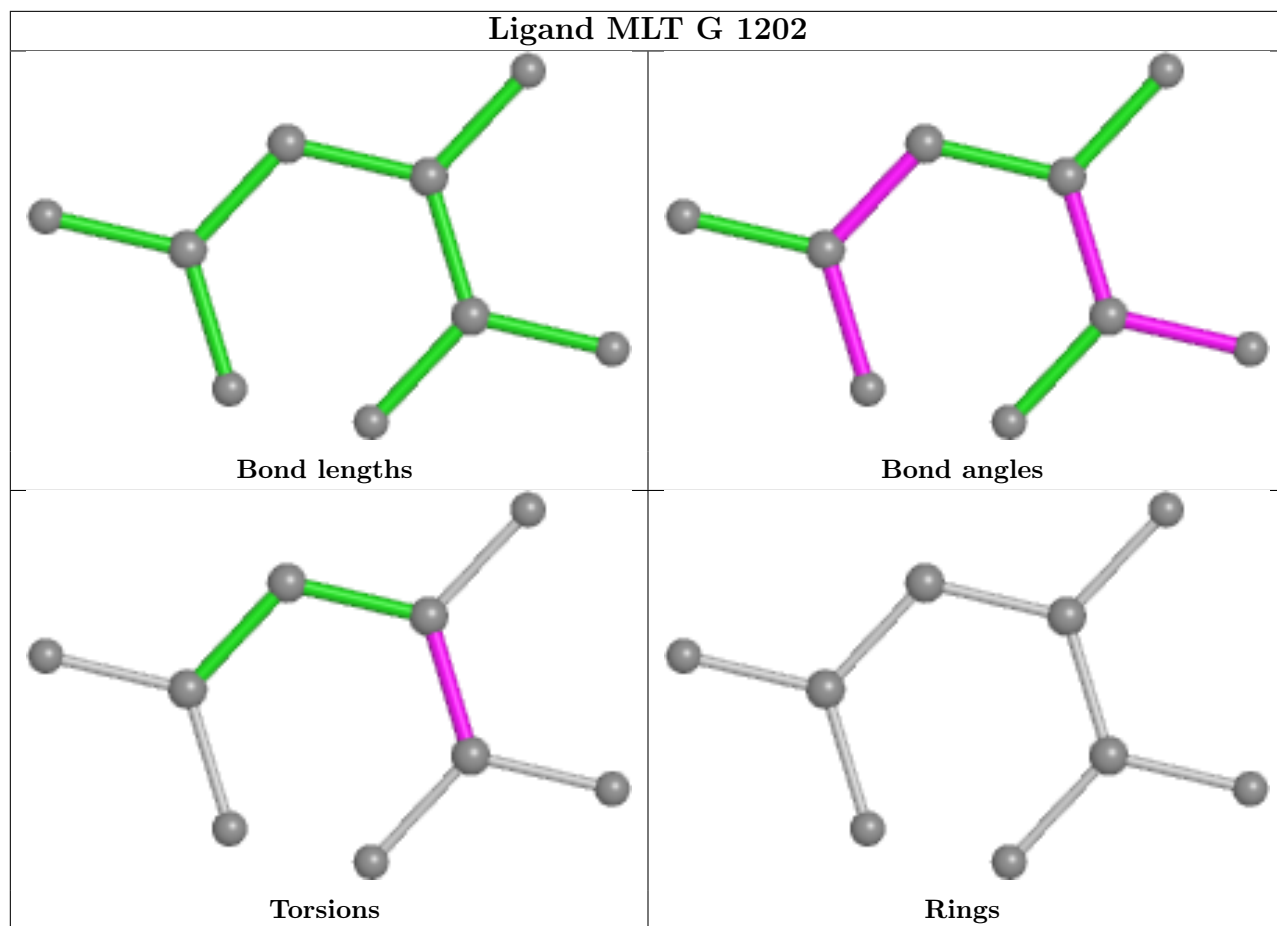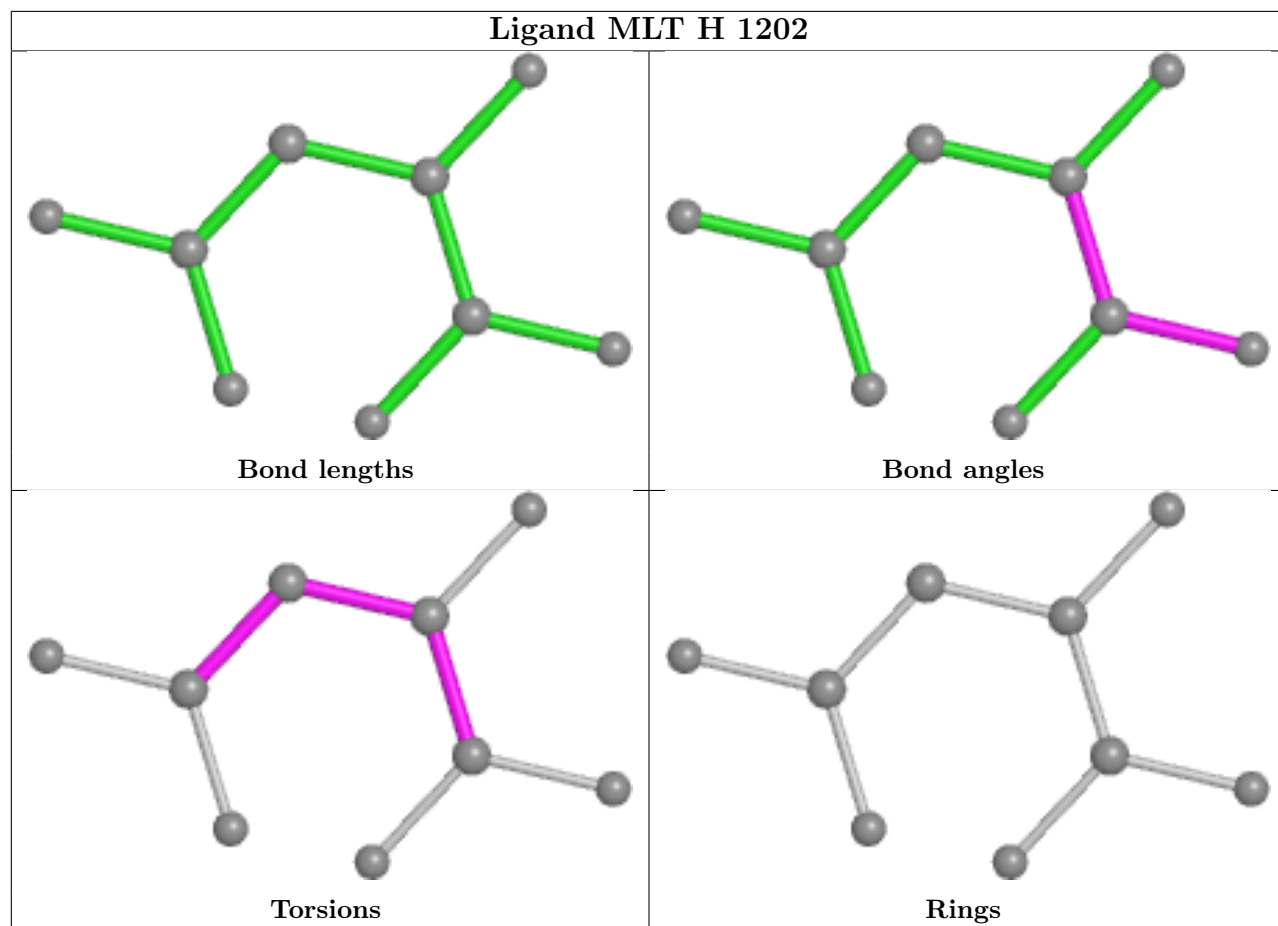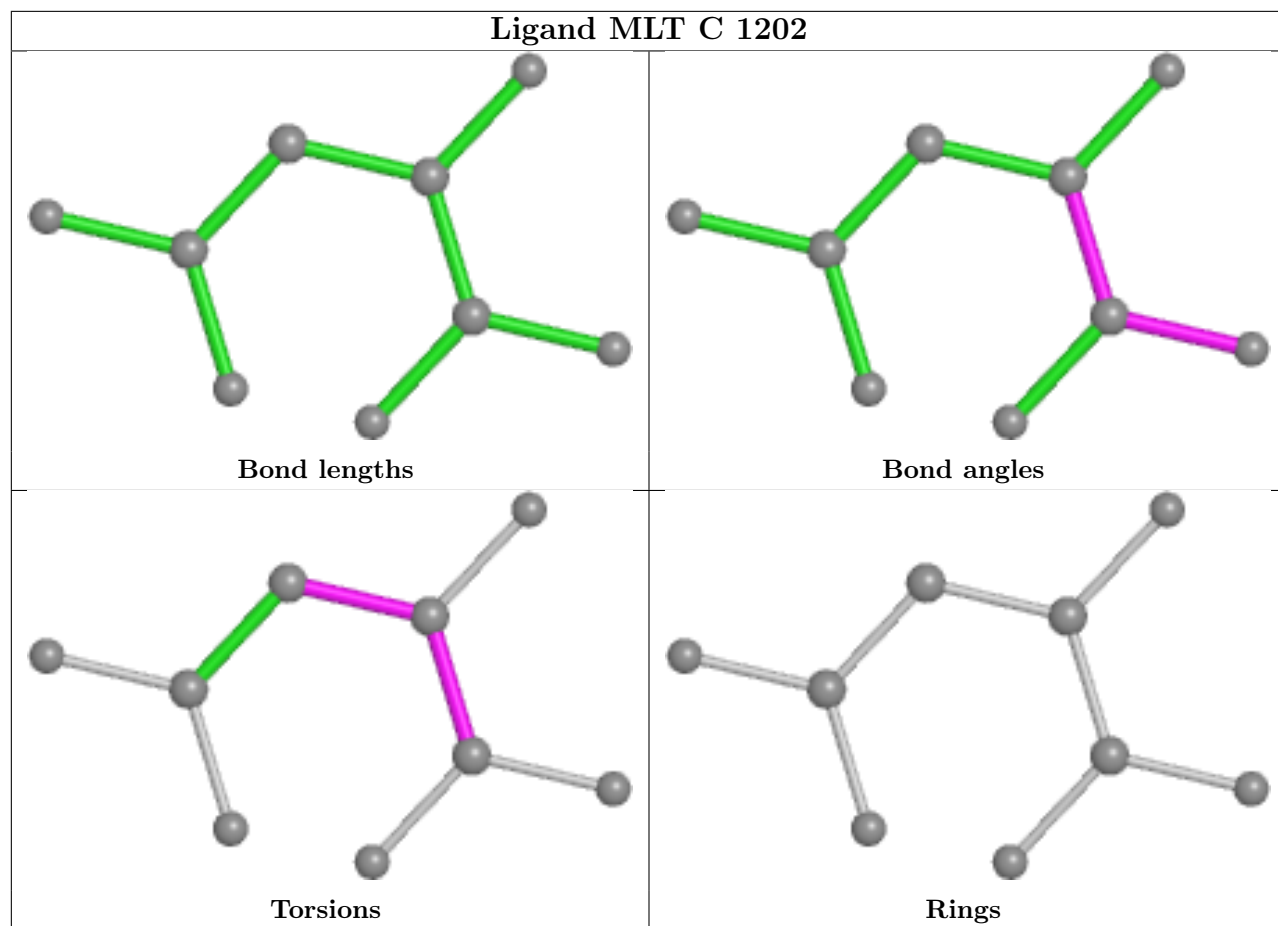
5.7 Other polymers (i)

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	1126/1131 (99%)	-0.08	5 (0%)	92	93	31, 49, 78, 145	0
1	B	1125/1131 (99%)	0.18	59 (5%)	27	24	33, 53, 121, 185	0
1	C	1125/1131 (99%)	-0.01	10 (0%)	84	83	31, 49, 94, 161	0
1	D	1124/1131 (99%)	-0.05	6 (0%)	91	91	32, 48, 86, 138	0
1	E	1120/1131 (99%)	0.04	16 (1%)	75	73	30, 52, 101, 175	0
1	F	1117/1131 (98%)	-0.01	5 (0%)	92	93	28, 52, 78, 145	0
1	G	1115/1131 (98%)	0.03	11 (0%)	82	81	32, 54, 84, 121	0
1	H	1122/1131 (99%)	-0.04	6 (0%)	91	91	34, 48, 78, 141	0
All	All	8974/9048 (99%)	0.01	118 (1%)	77	75	28, 51, 88, 185	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	512	PHE	12.0
1	B	526	HIS	6.9
1	B	546	SER	5.9
1	B	551	ASP	5.5
1	C	850	THR	5.4

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
3	MLT	C	1202	9/9	0.67	0.40	43,48,54,56	9
3	MLT	B	1202	9/9	0.87	0.33	52,54,56,56	9
3	MLT	G	1202	9/9	0.88	0.26	43,48,50,51	9
3	MLT	F	1202	9/9	0.91	0.24	35,38,40,42	9
3	MLT	A	1202	9/9	0.92	0.21	37,41,42,42	9
3	MLT	H	1202	9/9	0.93	0.19	42,43,46,46	9
2	MG	C	1201	1/1	0.94	0.28	42,42,42,42	0
2	MG	F	1201	1/1	0.94	0.15	32,32,32,32	0
2	MG	B	1201	1/1	0.96	0.19	33,33,33,33	0
2	MG	E	1201	1/1	0.97	0.19	29,29,29,29	0
2	MG	A	1201	1/1	0.97	0.18	31,31,31,31	0
2	MG	H	1201	1/1	0.98	0.19	32,32,32,32	0
2	MG	G	1201	1/1	0.99	0.22	31,31,31,31	0
2	MG	D	1201	1/1	0.99	0.19	33,33,33,33	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.
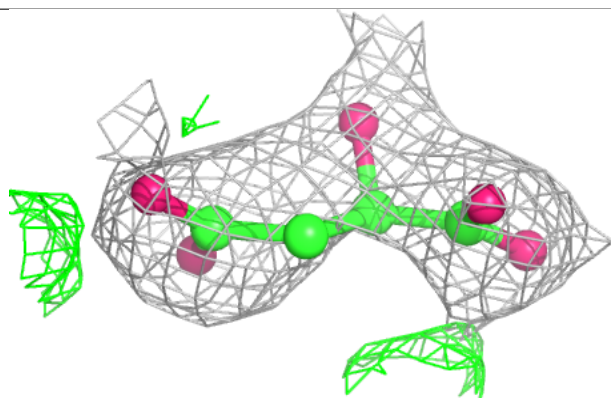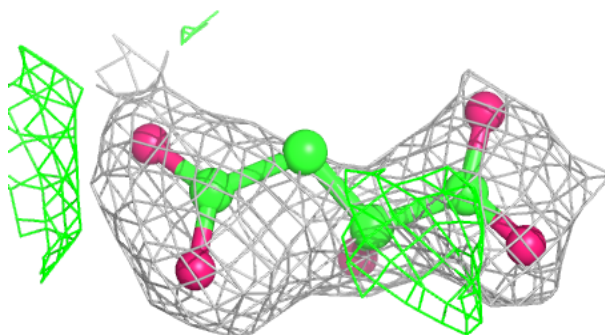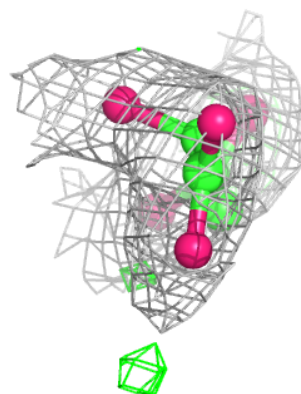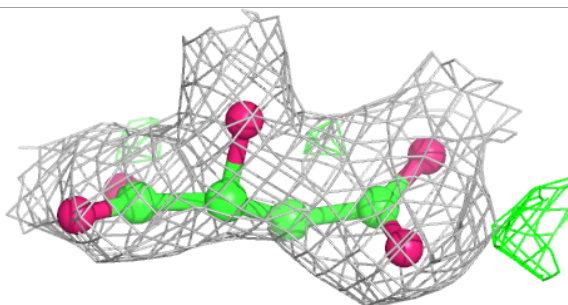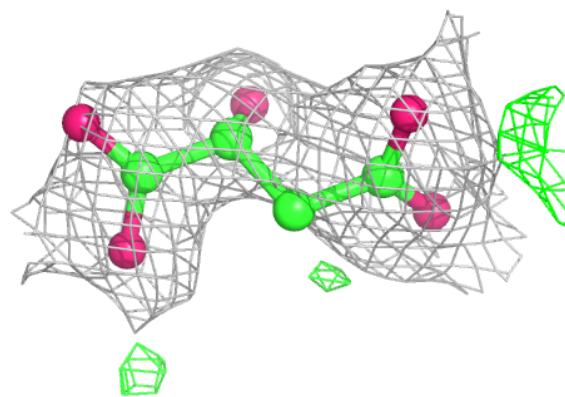
Electron density around MLT C 1202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
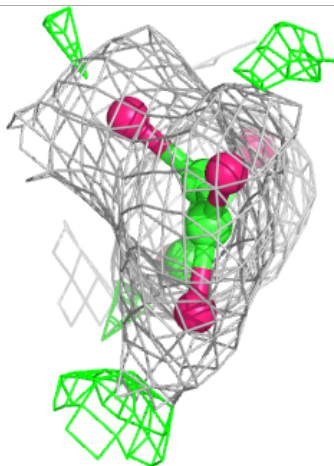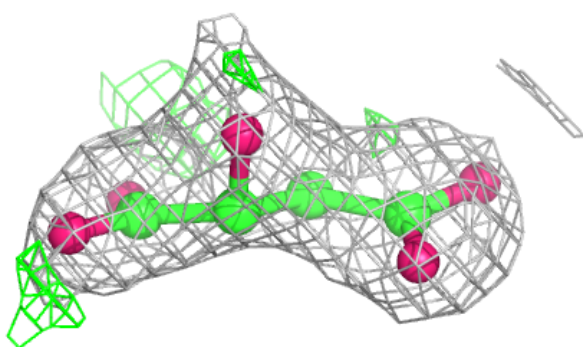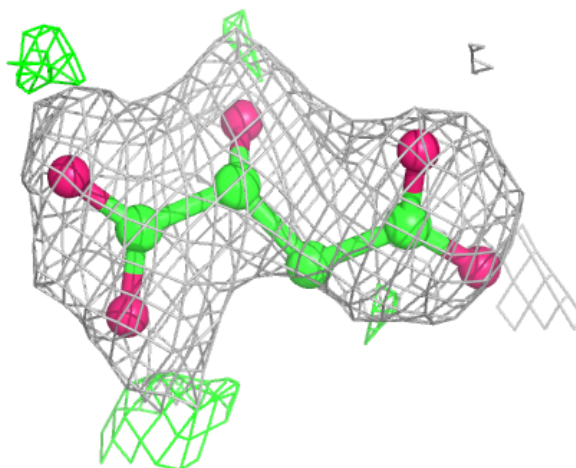mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
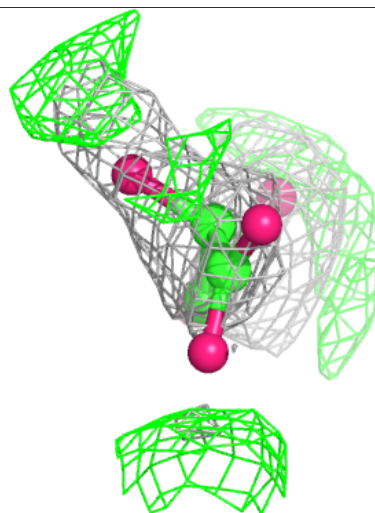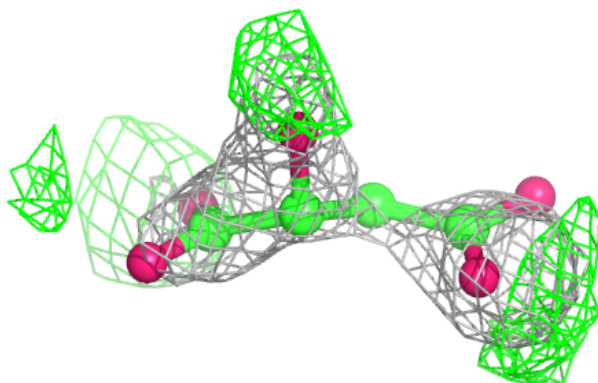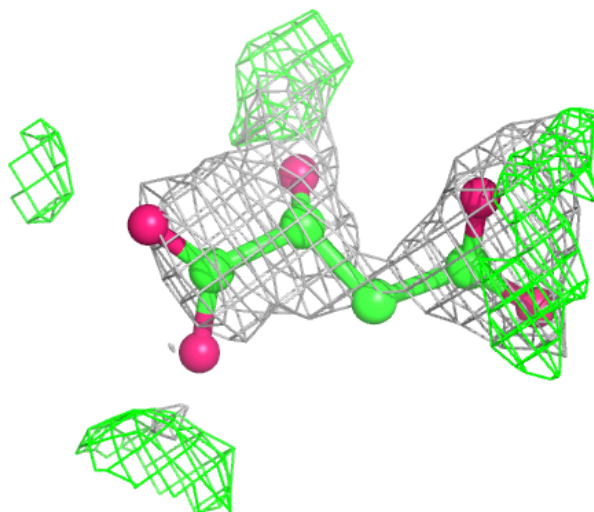
Electron density around MLT B 1202:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
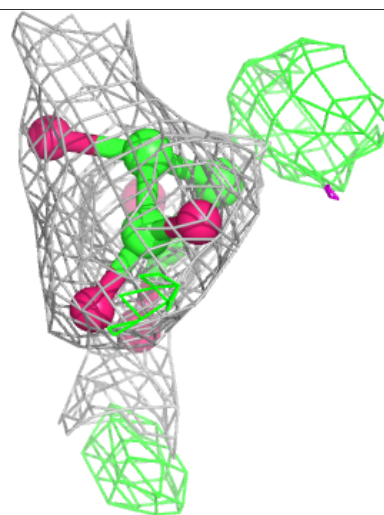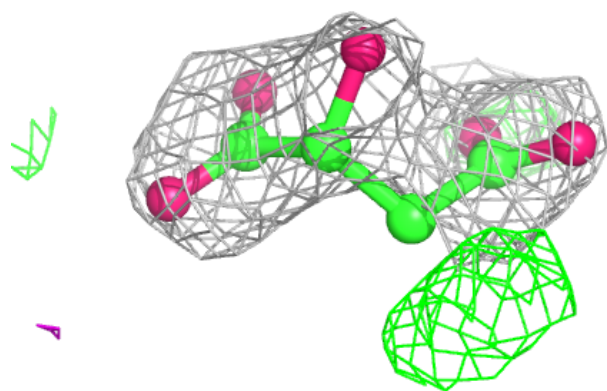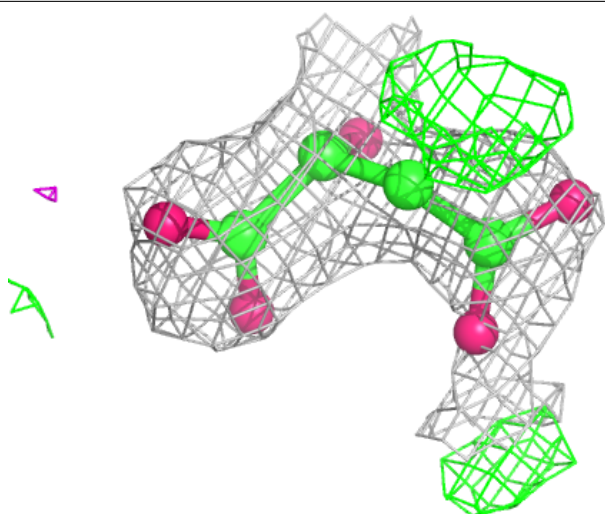
Electron density around MLT G 1202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
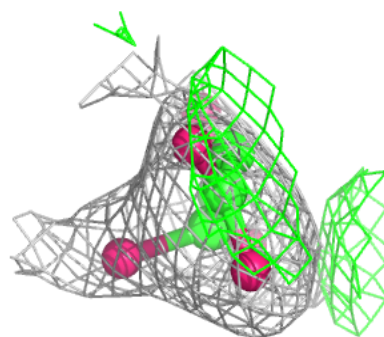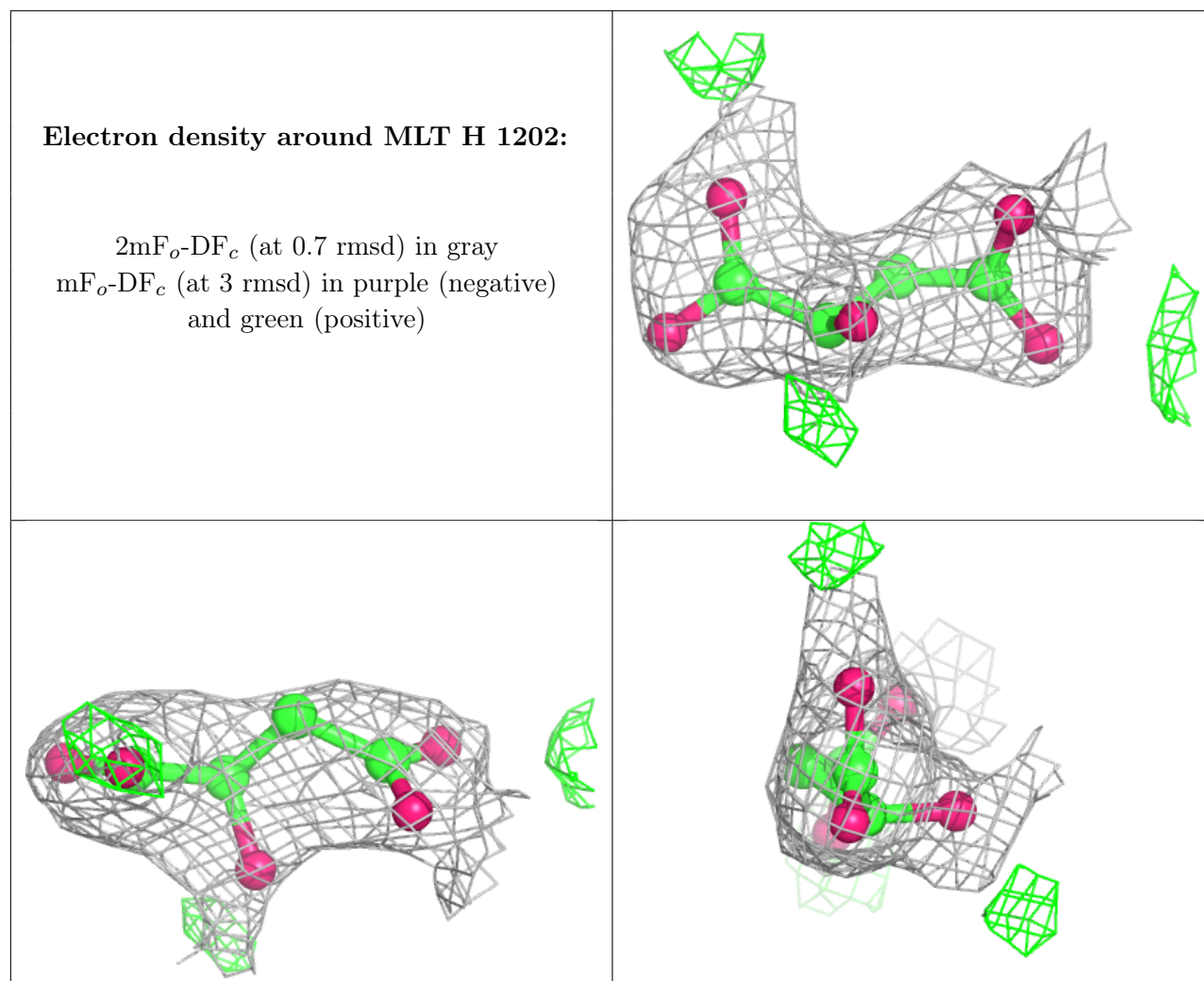
Electron density around MLT F 1202:

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

Electron density around MLT A 1202:

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

Electron density around MLT H 1202:

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

6.5 Other polymers (i)

There are no such residues in this entry.