Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:28 am BST

PDB ID	:	6HJX
Title	:	X-ray structure of a pentameric ligand gated ion channel from Erwinia chrysanthemi (ELIC) 7'C pore mutant (L238C) in complex with nanobody 72
Authors	:	Spurny, R.; Govaerts, C.; Evans, G.L.; Pardon, E.; Steyaert, J.; Ulens, C.
Deposited on	:	2018-09-04
Resolution	:	2.50 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	:	2.11
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)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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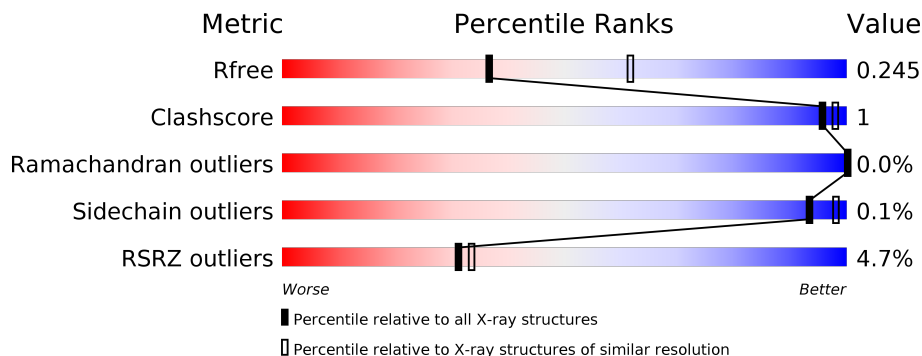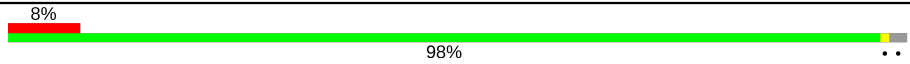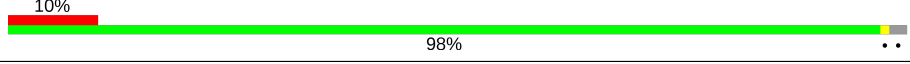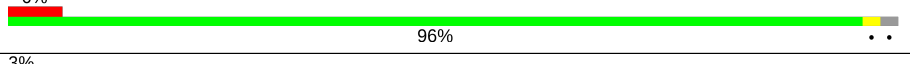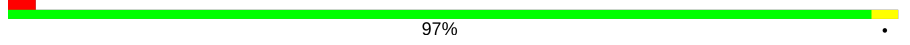

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	306	2% / 96%
2	B	309	3% / 95% / 5%
3	C	312	3% / 94%
4	D	310	5% / 95%
5	E	307	5% / 96%
6	F	124	6% / 98%

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Mol	Chain	Length	Quality of chain
6	G	124	
6	H	124	
6	I	124	
6	J	124	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 17226 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 Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total 2456	C 1602	N 408	O 441	S 5	0	3	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	insertion	UNP P0C7B7
A	238	CYS	LEU	engineered mutation	UNP P0C7B7
A	289	ASN	MET	conflict	UNP P0C7B7
A	300	SER	CYS	engineered mutation	UNP P0C7B7
A	313	SER	CYS	engineered mutation	UNP P0C7B7

- Molecule 2 is a protein called Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	309	Total 2489	C 1619	N 414	O 451	S 5	0	3	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	PRO	-	expression tag	UNP P0C7B7
B	7	VAL	-	expression tag	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	238	CYS	LEU	engineered mutation	UNP P0C7B7
B	289	ASN	MET	conflict	UNP P0C7B7
B	300	SER	CYS	engineered mutation	UNP P0C7B7
B	313	SER	CYS	engineered mutation	UNP P0C7B7

- Molecule 3 is a protein called Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	305	Total 2455	C 1603	N 404	O 443	S 5	0	1	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	6	PRO	-	expression tag	UNP P0C7B7
C	7	VAL	-	expression tag	UNP P0C7B7
C	164	GLY	-	insertion	UNP P0C7B7
C	238	CYS	LEU	engineered mutation	UNP P0C7B7
C	289	ASN	MET	conflict	UNP P0C7B7
C	300	SER	CYS	engineered mutation	UNP P0C7B7
C	313	SER	CYS	engineered mutation	UNP P0C7B7

- Molecule 4 is a protein called Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	302	Total 2402	C 1567	N 397	O 433	S 5	0	1	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	164	GLY	-	insertion	UNP P0C7B7
D	238	CYS	LEU	engineered mutation	UNP P0C7B7
D	289	ASN	MET	conflict	UNP P0C7B7
D	300	SER	CYS	engineered mutation	UNP P0C7B7
D	313	SER	CYS	engineered mutation	UNP P0C7B7

- Molecule 5 is a protein called Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	299	Total 2389	C 1561	N 388	O 435	S 5	0	1	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	164	GLY	-	insertion	UNP P0C7B7
E	238	CYS	LEU	engineered mutation	UNP P0C7B7
E	289	ASN	MET	conflict	UNP P0C7B7
E	300	SER	CYS	engineered mutation	UNP P0C7B7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	313	SER	CYS	engineered mutation	UNP P0C7B7

- Molecule 6 is a protein called nanobody 72.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	124	Total 898	C 559	N 161	O 173	S 5	0	0	0
6	G	122	Total 886	C 551	N 159	O 171	S 5	0	0	0
6	H	122	Total 884	C 549	N 158	O 172	S 5	0	0	0
6	I	121	Total 872	C 543	N 156	O 168	S 5	0	0	0
6	J	124	Total 885	C 549	N 159	O 172	S 5	0	0	0

- Molecule 7 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).
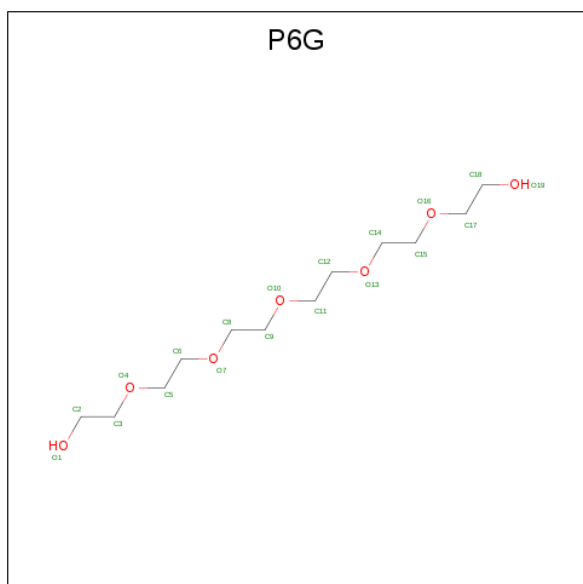
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 19	C 12	O 7	0	0
7	B	1	Total 19	C 12	O 7	0	0
7	D	1	Total 19	C 12	O 7	0	0
7	E	1	Total 19	C 12	O 7	0	0

- Molecule 8 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by author).
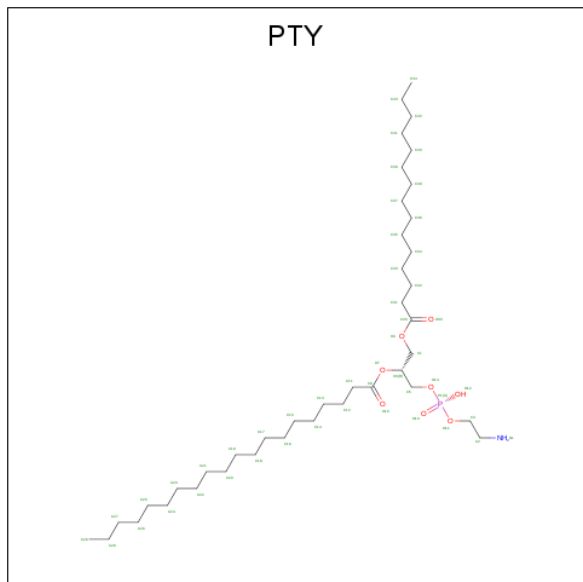
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	A	1	38	28	1	8	1	0	0

- Molecule 9 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).
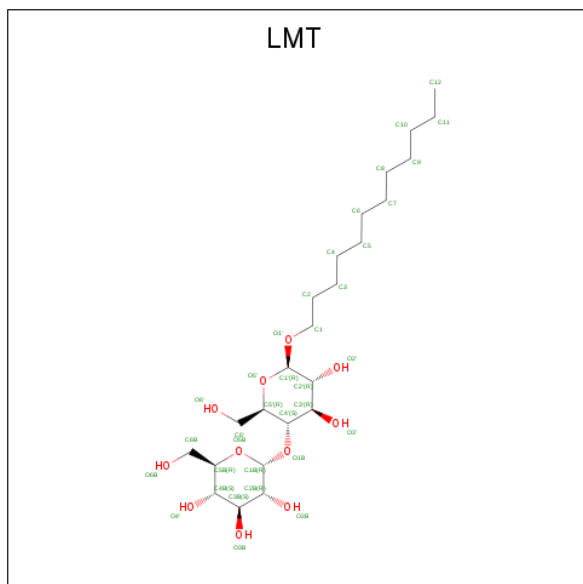
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	32	21	11	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total 35	C 24	O 11	0	0
9	C	1	Total 32	C 21	O 11	0	0
9	D	1	Total 32	C 21	O 11	0	0
9	E	1	Total 32	C 21	O 11	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).
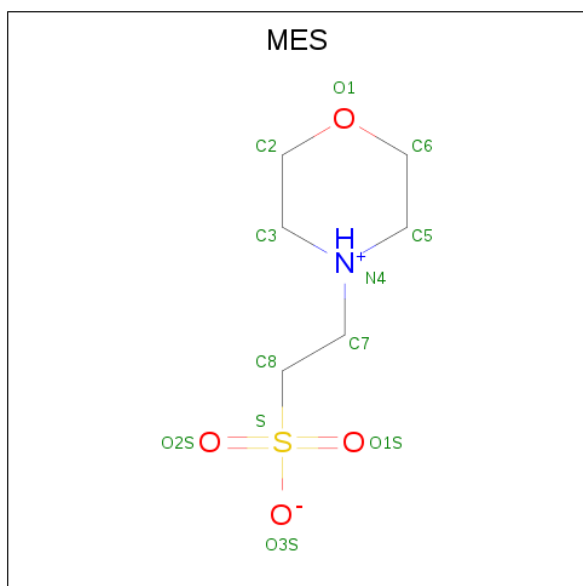
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total 24	C 12	N 2	O 8	S 2	0	1

- Molecule 11 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	1	Total 1	Na 1	0	0

- Molecule 12 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	55	Total 55	O 55	0	0
12	B	59	Total 59	O 59	0	0
12	C	48	Total 48	O 48	0	0
12	D	41	Total 41	O 41	0	0
12	E	42	Total 42	O 42	0	0
12	F	21	Total 21	O 21	0	0
12	G	10	Total 10	O 10	0	0
12	H	13	Total 13	O 13	0	0
12	I	12	Total 12	O 12	0	0
12	J	7	Total 7	O 7	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
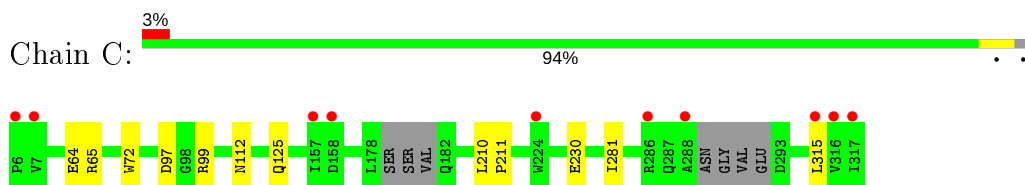
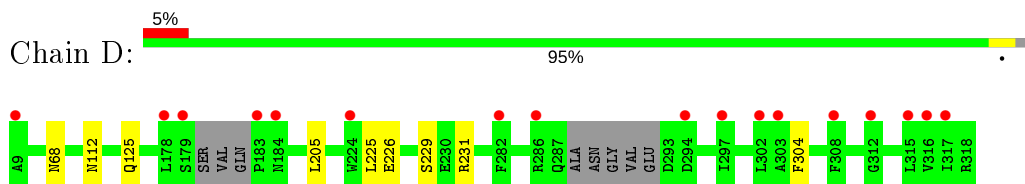- Molecule 1: Cys-loop ligand-gated ion channel
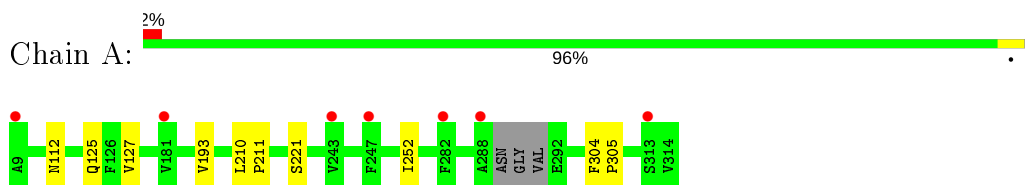
- Molecule 2: Cys-loop ligand-gated ion channel
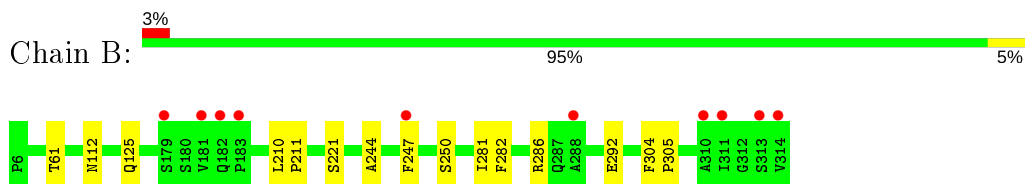
- Molecule 3: Cys-loop ligand-gated ion channel

- Molecule 4: Cys-loop ligand-gated ion channel

- Molecule 5: Cys-loop ligand-gated ion channel
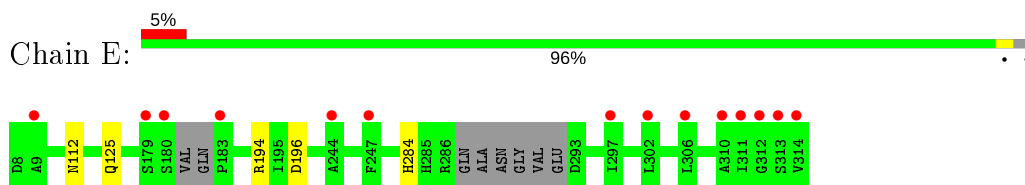
- Molecule 6: nanobody 72
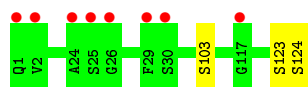
Chain F:

6%

98%

Q1 V2 A24 S25 G26 F29 S30 S103 G117 S123 S124

● Molecule 6: nanobody 72

Chain G:

8%

98%

GLN VAL Q3 A24 R27 I28 F29 S30 M78 I100 S103 Y113 W114 G115 Q116 S124

● Molecule 6: nanobody 72

Chain H:

10%

98%

GLN V2 Q3 E6 L18 A24 S25 G26 R27 I28 F29 A75 K76 N77 G101 Y113 S123 SER

● Molecule 6: nanobody 72

Chain I:

6%

96%

GLN VAL Q3 Q13 A14 A24 S25 G26 R27 I28 F29 E89 S103 V122 S123 SER

● Molecule 6: nanobody 72

Chain J:

3%

97%

Q1 V2 E6 F29 F37 I54 Y95 S103 S124
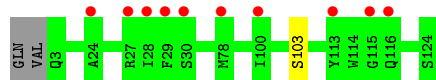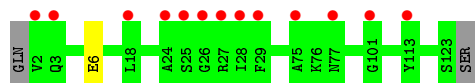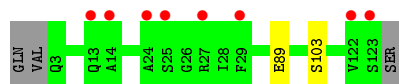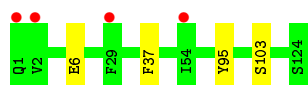
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.25Å　156.28Å　102.50Å 90.00°　102.88°　90.00°	Depositor
Resolution (Å)	47.59　–　2.50 48.50　–　2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.59-2.50) 99.8 (48.50-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.41 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.204　,　0.245 0.204　,　0.245	Depositor DCC
R_{free} test set	5070 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.3	EDS
L-test for twinning [2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17226	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: NA, P6G, LMT, PTY, MES

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	0/2528	0.42	0/3450
2	B	0.25	0/2562	0.42	0/3498
3	C	0.25	0/2522	0.41	0/3444
4	D	0.25	0/2469	0.42	0/3373
5	E	0.25	0/2458	0.42	0/3357
6	F	0.27	0/914	0.47	0/1238
6	G	0.25	0/902	0.46	0/1221
6	H	0.26	0/900	0.46	0/1220
6	I	0.27	0/888	0.46	0/1204
6	J	0.26	0/901	0.45	0/1222
All	All	0.25	0/17044	0.43	0/23227

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	2456	0	2373	7	0
2	B	2489	0	2391	10	0
3	C	2455	0	2379	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2402	0	2285	6	0
5	E	2389	0	2296	5	0
6	F	898	0	846	2	0
6	G	886	0	832	1	0
6	H	884	0	820	1	0
6	I	872	0	810	2	0
6	J	885	0	813	3	0
7	A	19	0	26	0	0
7	B	19	0	26	0	0
7	D	19	0	26	0	0
7	E	19	0	26	0	0
8	A	38	0	49	0	0
9	A	32	0	36	0	0
9	B	35	0	46	0	0
9	C	32	0	37	1	0
9	D	32	0	37	0	0
9	E	32	0	37	0	0
10	C	24	0	26	1	0
11	C	1	0	0	0	0
12	A	55	0	0	0	0
12	B	59	0	0	0	0
12	C	48	0	0	0	0
12	D	41	0	0	0	0
12	E	42	0	0	0	0
12	F	21	0	0	0	0
12	G	10	0	0	0	0
12	H	13	0	0	0	0
12	I	12	0	0	0	0
12	J	7	0	0	0	0
All	All	17226	0	16217	36	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 1.

All (36) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112[B]:ASN:OD1	6:F:103:SER:OG	1.92	0.86
3:C:230:GLU:OE2	4:D:229:SER:OG	1.95	0.84
5:E:112[A]:ASN:OD1	6:J:103:SER:OG	1.98	0.81
1:A:112[B]:ASN:ND2	1:A:125:GLN:O	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112[A]:ASN:ND2	2:B:125:GLN:O	2.18	0.76
3:C:112[B]:ASN:ND2	3:C:125:GLN:O	2.19	0.74
2:B:61:THR:OG1	3:C:64:GLU:OE2	2.14	0.64
2:B:112[A]:ASN:OD1	6:G:103:SER:OG	2.04	0.62
6:J:6:GLU:OE1	6:J:6:GLU:N	2.35	0.59
5:E:112[A]:ASN:ND2	5:E:125:GLN:O	2.36	0.58
4:D:225:LEU:O	4:D:231:ARG:NH1	2.33	0.56
4:D:112:ASN:ND2	4:D:125:GLN:O	2.39	0.55
4:D:226:GLU:OE1	5:E:284:HIS:NE2	2.41	0.50
2:B:282:PHE:O	2:B:286:ARG:N	2.45	0.49
5:E:194:ARG:NH1	5:E:196:ASP:OD1	2.46	0.47
4:D:112:ASN:ND2	6:I:103:SER:OG	2.45	0.47
2:B:304:PHE:HB3	2:B:305:PRO:HD3	1.96	0.46
6:I:89:GLU:OE1	6:I:89:GLU:N	2.46	0.45
1:A:221:SER:HB2	2:B:281:ILE:HD11	1.99	0.45
3:C:315:LEU:HD11	9:C:401:LMT:H51	1.98	0.45
6:J:37:PHE:O	6:J:95:TYR:N	2.44	0.43
2:B:244:ALA:HA	2:B:247[B]:PHE:CE2	2.54	0.43
2:B:221:SER:HB2	3:C:281:ILE:HD11	2.01	0.43
3:C:65:ARG:NH1	4:D:68:ASN:O	2.52	0.43
1:A:304:PHE:HB3	1:A:305:PRO:HD3	2.01	0.42
5:E:112[B]:ASN:ND2	5:E:125:GLN:O	2.53	0.41
1:A:252:ILE:HD11	2:B:250:SER:HB2	2.02	0.41
3:C:112[A]:ASN:ND2	3:C:125:GLN:O	2.53	0.41
1:A:210:LEU:HB3	1:A:211:PRO:HD3	2.02	0.41
3:C:72:TRP:NE1	10:C:402[B]:MES:O3S	2.53	0.41
3:C:210:LEU:HB3	3:C:211:PRO:HD3	2.03	0.41
6:F:123:SER:O	6:F:124:SER:CB	2.69	0.41
1:A:127:VAL:HA	1:A:193:VAL:O	2.20	0.41
2:B:210:LEU:HB3	2:B:211:PRO:HD3	2.02	0.41
3:C:97:ASP:OD2	3:C:99:ARG:NH2	2.51	0.40
6:H:6:GLU:OE1	6:H:6:GLU:N	2.49	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	302/306 (99%)	293 (97%)	9 (3%)	0	100	100
2	B	310/309 (100%)	298 (96%)	11 (4%)	1 (0%)	41	61
3	C	300/312 (96%)	285 (95%)	15 (5%)	0	100	100
4	D	297/310 (96%)	286 (96%)	11 (4%)	0	100	100
5	E	294/307 (96%)	286 (97%)	8 (3%)	0	100	100
6	F	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
6	G	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
6	H	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
6	I	119/124 (96%)	112 (94%)	7 (6%)	0	100	100
6	J	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
All	All	2106/2164 (97%)	2022 (96%)	83 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	292	GLU

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	262/273 (96%)	262 (100%)	0	100	100
2	B	264/276 (96%)	264 (100%)	0	100	100
3	C	263/279 (94%)	263 (100%)	0	100	100
4	D	251/277 (91%)	249 (99%)	2 (1%)	81	93
5	E	255/274 (93%)	255 (100%)	0	100	100
6	F	87/96 (91%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	86/96 (90%)	86 (100%)	0	100	100
6	H	85/96 (88%)	85 (100%)	0	100	100
6	I	83/96 (86%)	83 (100%)	0	100	100
6	J	83/96 (86%)	83 (100%)	0	100	100
All	All	1719/1859 (92%)	1717 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	205	LEU
4	D	304	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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
10	MES	C	402[B]	-	12,12,12	1.40	3 (25%)	14,16,16	2.05	4 (28%)
9	LMT	E	401	-	33,33,36	1.16	5 (15%)	44,44,47	1.01	2 (4%)
9	LMT	A	503	-	33,33,36	1.19	5 (15%)	44,44,47	0.95	1 (2%)
9	LMT	C	401	-	33,33,36	1.16	5 (15%)	44,44,47	1.01	2 (4%)
7	P6G	D	402	-	18,18,18	0.53	0	17,17,17	0.34	0
7	P6G	E	402	-	18,18,18	0.53	0	17,17,17	0.34	0
7	P6G	A	501	-	18,18,18	0.53	0	17,17,17	0.32	0
10	MES	C	402[A]	-	12,12,12	1.40	3 (25%)	14,16,16	1.91	4 (28%)
9	LMT	B	401	-	36,36,36	1.13	5 (13%)	47,47,47	1.00	2 (4%)
7	P6G	B	402	-	18,18,18	0.53	0	17,17,17	0.27	0
8	PTY	A	502	-	37,37,49	0.99	4 (10%)	40,42,54	1.12	2 (5%)
9	LMT	D	401	-	33,33,36	1.15	5 (15%)	44,44,47	1.07	2 (4%)

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
10	MES	C	402[B]	-	-	1/6/14/14	0/1/1/1
9	LMT	E	401	-	-	7/18/58/61	0/2/2/2
9	LMT	A	503	-	-	6/18/58/61	0/2/2/2
9	LMT	C	401	-	-	5/18/58/61	0/2/2/2
7	P6G	D	402	-	-	8/16/16/16	-
7	P6G	E	402	-	-	9/16/16/16	-
7	P6G	A	501	-	-	9/16/16/16	-
10	MES	C	402[A]	-	-	4/6/14/14	0/1/1/1
9	LMT	B	401	-	-	5/21/61/61	0/2/2/2
7	P6G	B	402	-	-	6/16/16/16	-
8	PTY	A	502	-	-	21/41/41/53	-
9	LMT	D	401	-	-	7/18/58/61	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	402[B]	MES	C8-S	3.30	1.82	1.77
10	C	402[A]	MES	C8-S	3.21	1.82	1.77
9	A	503	LMT	O3'-C3'	-2.68	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	401	LMT	O3'-C3'	-2.58	1.36	1.43
9	B	401	LMT	O3'-C3'	-2.54	1.37	1.43
9	D	401	LMT	O3'-C3'	-2.53	1.37	1.43
9	E	401	LMT	O3'-C3'	-2.50	1.37	1.43
8	A	502	PTY	O7-C6	-2.48	1.40	1.46
9	B	401	LMT	O2'-C2'	-2.47	1.37	1.43
9	C	401	LMT	O2'-C2'	-2.44	1.37	1.43
9	A	503	LMT	O2B-C2B	-2.43	1.37	1.43
9	E	401	LMT	O2'-C2'	-2.43	1.37	1.43
8	A	502	PTY	O4-C30	2.39	1.40	1.33
9	E	401	LMT	O3B-C3B	-2.35	1.37	1.43
9	A	503	LMT	O3B-C3B	-2.32	1.37	1.43
9	A	503	LMT	O2'-C2'	-2.32	1.37	1.43
9	C	401	LMT	O3B-C3B	-2.32	1.37	1.43
9	C	401	LMT	O2B-C2B	-2.31	1.37	1.43
9	E	401	LMT	O2B-C2B	-2.30	1.37	1.43
9	D	401	LMT	O2'-C2'	-2.27	1.37	1.43
9	B	401	LMT	O3B-C3B	-2.26	1.37	1.43
9	D	401	LMT	O2B-C2B	-2.24	1.37	1.43
9	D	401	LMT	O3B-C3B	-2.23	1.37	1.43
9	B	401	LMT	O2B-C2B	-2.23	1.37	1.43
10	C	402[A]	MES	O1S-S	2.23	1.51	1.45
10	C	402[B]	MES	O2S-S	2.21	1.51	1.45
10	C	402[A]	MES	O2S-S	2.19	1.51	1.45
10	C	402[B]	MES	O1S-S	2.17	1.51	1.45
8	A	502	PTY	O7-C8	2.14	1.40	1.34
9	C	401	LMT	O4'-C4B	-2.11	1.38	1.43
9	E	401	LMT	O4'-C4B	-2.08	1.38	1.43
9	B	401	LMT	O4'-C4B	-2.08	1.38	1.43
9	D	401	LMT	O4'-C4B	-2.06	1.38	1.43
8	A	502	PTY	O4-C1	-2.06	1.40	1.45
9	A	503	LMT	O4'-C4B	-2.03	1.38	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	402[B]	MES	O2S-S-C8	4.31	112.11	106.92
10	C	402[B]	MES	O1S-S-C8	4.13	111.89	106.92
8	A	502	PTY	O7-C8-C11	3.97	120.05	111.50
10	C	402[B]	MES	O2S-S-O1S	-3.84	100.64	113.95
10	C	402[A]	MES	O2S-S-O1S	-3.82	100.72	113.95
10	C	402[A]	MES	O2S-S-C8	3.63	111.29	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	402[A]	MES	O1S-S-C8	3.55	111.19	106.92
10	C	402[A]	MES	O3S-S-C8	2.97	110.57	105.77
8	A	502	PTY	O4-C30-C31	2.64	120.19	111.91
9	D	401	LMT	O5B-C5B-C4B	2.64	114.48	109.69
9	E	401	LMT	C1'-O5'-C5'	-2.61	108.57	113.69
10	C	402[B]	MES	O3S-S-C8	2.55	109.89	105.77
9	B	401	LMT	C1'-O5'-C5'	-2.47	108.85	113.69
9	D	401	LMT	C1'-O5'-C5'	-2.40	108.98	113.69
9	A	503	LMT	C1'-O5'-C5'	-2.34	109.09	113.69
9	C	401	LMT	C1'-O5'-C5'	-2.27	109.24	113.69
9	B	401	LMT	C3B-C4B-C5B	-2.26	106.21	110.24
9	C	401	LMT	O5B-C5B-C4B	2.16	113.62	109.69
9	E	401	LMT	O5B-C5B-C4B	2.13	113.57	109.69

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	402[B]	MES	N4-C7-C8-S
9	C	401	LMT	C2-C1-O1'-C1'
10	C	402[A]	MES	N4-C7-C8-S
9	B	401	LMT	C2'-C1'-O1'-C1
9	B	401	LMT	O5'-C1'-O1'-C1
8	A	502	PTY	N1-C2-C3-O11
8	A	502	PTY	C11-C8-O7-C6
8	A	502	PTY	C3-O11-P1-O12
8	A	502	PTY	C3-O11-P1-O13
8	A	502	PTY	C3-O11-P1-O14
8	A	502	PTY	C5-O14-P1-O13
8	A	502	PTY	O10-C8-O7-C6
8	A	502	PTY	C31-C30-O4-C1
8	A	502	PTY	O30-C30-O4-C1
7	A	501	P6G	O13-C14-C15-O16
7	D	402	P6G	O13-C14-C15-O16
7	B	402	P6G	O10-C11-C12-O13
9	D	401	LMT	C4'-C5'-C6'-O6'
9	D	401	LMT	O5'-C5'-C6'-O6'
7	B	402	P6G	O13-C14-C15-O16
7	D	402	P6G	O4-C5-C6-O7
9	C	401	LMT	O1'-C1-C2-C3
9	E	401	LMT	O1'-C1-C2-C3
10	C	402[A]	MES	C7-C8-S-O3S

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Mol	Chain	Res	Type	Atoms
9	A	503	LMT	O1'-C1-C2-C3
7	E	402	P6G	O1-C2-C3-O4
8	A	502	PTY	C14-C15-C16-C17
8	A	502	PTY	C31-C32-C33-C34
9	D	401	LMT	O5B-C5B-C6B-O6B
9	C	401	LMT	C1-C2-C3-C4
9	A	503	LMT	C4'-C5'-C6'-O6'
9	E	401	LMT	C1-C2-C3-C4
9	A	503	LMT	O5B-C5B-C6B-O6B
9	D	401	LMT	C5-C6-C7-C8
8	A	502	PTY	C5-O14-P1-O11
9	A	503	LMT	C1-C2-C3-C4
7	A	501	P6G	O1-C2-C3-O4
9	B	401	LMT	C5'-C4'-O1B-C1B
8	A	502	PTY	O4-C1-C6-O7
8	A	502	PTY	C11-C12-C13-C14
9	D	401	LMT	O5'-C1'-O1'-C1
9	D	401	LMT	C2-C1-O1'-C1'
9	A	503	LMT	O5'-C5'-C6'-O6'
9	C	401	LMT	C5-C6-C7-C8
9	E	401	LMT	O5'-C1'-O1'-C1
9	D	401	LMT	O1'-C1-C2-C3
7	A	501	P6G	O4-C5-C6-O7
7	E	402	P6G	C12-C11-O10-C9
7	D	402	P6G	C9-C8-O7-C6
7	D	402	P6G	C2-C3-O4-C5
8	A	502	PTY	C6-C5-O14-P1
7	A	501	P6G	C8-C9-O10-C11
7	D	402	P6G	O7-C8-C9-O10
7	B	402	P6G	C9-C8-O7-C6
7	E	402	P6G	C9-C8-O7-C6
9	B	401	LMT	C3'-C4'-O1B-C1B
9	E	401	LMT	C5-C6-C7-C8
8	A	502	PTY	C5-O14-P1-O12
10	C	402[A]	MES	C7-C8-S-O2S
8	A	502	PTY	C2-C3-O11-P1
7	E	402	P6G	C11-C12-O13-C14
7	A	501	P6G	C6-C5-O4-C3
8	A	502	PTY	O4-C1-C6-C5
7	B	402	P6G	C8-C9-O10-C11
7	A	501	P6G	C9-C8-O7-C6
7	A	501	P6G	C18-C17-O16-C15

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Mol	Chain	Res	Type	Atoms
8	A	502	PTY	C12-C11-C8-O7
9	E	401	LMT	C2'-C1'-O1'-C1
7	A	501	P6G	C5-C6-O7-C8
7	E	402	P6G	C14-C15-O16-C17
8	A	502	PTY	C33-C34-C35-C36
7	D	402	P6G	C12-C11-O10-C9
7	D	402	P6G	C8-C9-O10-C11
7	A	501	P6G	O16-C17-C18-O19
9	B	401	LMT	O5B-C1B-O1B-C4'
8	A	502	PTY	C18-C19-C20-C21
9	E	401	LMT	O5B-C1B-O1B-C4'
7	E	402	P6G	C8-C9-O10-C11
7	E	402	P6G	O4-C5-C6-O7
7	E	402	P6G	O10-C11-C12-O13
7	D	402	P6G	O10-C11-C12-O13
9	E	401	LMT	C2B-C1B-O1B-C4'
9	C	401	LMT	C6-C7-C8-C9
7	E	402	P6G	O13-C14-C15-O16
10	C	402[A]	MES	C7-C8-S-O1S
7	B	402	P6G	C14-C15-O16-C17
7	B	402	P6G	C18-C17-O16-C15
9	A	503	LMT	C2-C1-O1'-C1'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	402[B]	MES	1	0
9	C	401	LMT	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 LMT E 401

Bond lengths

Bond angles

Torsions

Rings

Ligand LMT A 503

Bond lengths

Bond angles

Torsions

Rings

Ligand LMT C 401	
Bond lengths	Bond angles
Torsions	Rings

Ligand P6G D 402	
Bond lengths	Bond angles
Torsions	Rings

Ligand P6G E 402	
Bond lengths	Bond angles
Torsions	Rings

Ligand P6G A 501	
Bond lengths	Bond angles
Torsions	Rings

Ligand LMT B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand P6G B 402

Bond lengths

Bond angles

Torsions

Rings

Ligand PTY A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand LMT D 401

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 (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	303/306 (99%)	-0.01	7 (2%)	60	63	36, 53, 87, 112	0
2	B	309/309 (100%)	0.13	10 (3%)	47	51	34, 52, 92, 125	0
3	C	305/312 (97%)	0.05	10 (3%)	46	50	35, 54, 87, 118	0
4	D	302/310 (97%)	0.06	17 (5%)	24	25	36, 58, 94, 146	0
5	E	299/307 (97%)	-0.00	14 (4%)	31	33	37, 57, 90, 103	0
6	F	124/124 (100%)	0.07	8 (6%)	18	19	37, 51, 75, 88	0
6	G	122/124 (98%)	0.42	10 (8%)	11	11	43, 65, 90, 116	0
6	H	122/124 (98%)	0.33	13 (10%)	6	5	45, 72, 93, 111	0
6	I	121/124 (97%)	0.09	8 (6%)	18	19	41, 57, 86, 111	0
6	J	124/124 (100%)	0.02	4 (3%)	47	51	48, 67, 106, 118	0
All	All	2131/2164 (98%)	0.09	101 (4%)	31	33	34, 57, 91, 146	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	181	VAL	6.8
5	E	314	VAL	6.6
6	H	29	PHE	5.9
6	H	27	ARG	5.9
6	J	29	PHE	5.7
4	D	315	LEU	5.5
2	B	314	VAL	5.5
6	J	2	VAL	5.4
6	H	28	ILE	5.4
6	H	26	GLY	5.3
4	D	183	PRO	4.9
4	D	317	ILE	4.9
6	H	2	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
6	I	27	ARG	4.6
4	D	179	SER	4.6
5	E	179	SER	4.5
3	C	317	ILE	4.4
6	G	29	PHE	4.3
6	H	25	SER	4.2
6	G	24	ALA	4.1
6	G	100	ILE	3.8
5	E	306	LEU	3.7
4	D	282	PHE	3.6
2	B	313	SER	3.6
2	B	310	ALA	3.5
3	C	7	VAL	3.3
6	I	123	SER	3.3
6	F	29	PHE	3.3
6	F	1	GLN	3.3
4	D	286	ARG	3.3
6	G	78	MET	3.2
3	C	6	PRO	3.2
4	D	9	ALA	3.1
5	E	302	LEU	3.1
6	G	27	ARG	3.1
2	B	311	ILE	3.1
6	I	29	PHE	3.1
4	D	184	ASN	3.1
5	E	180	SER	3.1
6	I	122	VAL	3.0
2	B	179	SER	3.0
4	D	297	ILE	2.9
2	B	183	PRO	2.8
6	G	28	ILE	2.8
6	G	113	TYR	2.8
2	B	247[A]	PHE	2.8
5	E	311	ILE	2.8
6	H	24	ALA	2.8
3	C	157	ILE	2.7
2	B	288	ALA	2.7
6	F	26	GLY	2.6
1	A	181	VAL	2.6
6	H	77	ASN	2.6
6	J	1	GLN	2.6
4	D	316	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
6	H	101	GLY	2.5
6	F	25	SER	2.5
5	E	310	ALA	2.5
6	G	30	SER	2.5
5	E	183	PRO	2.5
5	E	312	GLY	2.5
6	I	25	SER	2.4
3	C	315	LEU	2.4
6	F	30	SER	2.4
4	D	178	LEU	2.4
6	G	116	GLN	2.4
4	D	303	ALA	2.4
3	C	316	VAL	2.4
6	H	3	GLN	2.3
3	C	288	ALA	2.3
5	E	313	SER	2.3
6	F	2	VAL	2.3
3	C	286	ARG	2.3
5	E	247	PHE	2.3
6	J	54	ILE	2.3
6	H	18	LEU	2.3
5	E	9	ALA	2.2
6	F	117	GLY	2.2
1	A	282	PHE	2.2
3	C	224	TRP	2.2
6	F	24	ALA	2.2
6	H	113	TYR	2.2
1	A	288	ALA	2.2
6	I	13	GLN	2.2
5	E	297	ILE	2.2
4	D	294	ASP	2.2
1	A	9	ALA	2.1
4	D	224	TRP	2.1
6	G	115	GLY	2.1
5	E	244	ALA	2.1
6	H	75	ALA	2.1
6	I	24	ALA	2.1
1	A	313	SER	2.1
4	D	312	GLY	2.1
6	I	14	ALA	2.0
4	D	302	LEU	2.0
3	C	158	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	182	GLN	2.0
1	A	243	VAL	2.0
1	A	247[A]	PHE	2.0
4	D	308	PHE	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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	P6G	E	402	19/19	0.77	0.24	67,81,90,92	0
10	MES	C	402[B]	12/12	0.78	0.23	52,58,63,65	12
10	MES	C	402[A]	12/12	0.78	0.23	56,62,66,70	12
8	PTY	A	502	38/50	0.78	0.35	66,93,117,127	0
9	LMT	D	401	32/35	0.79	0.34	69,102,130,133	0
11	NA	C	403	1/1	0.82	1.03	74,74,74,74	0
9	LMT	C	401	32/35	0.83	0.24	71,92,102,112	0
9	LMT	A	503	32/35	0.84	0.18	67,90,113,117	0
9	LMT	B	401	35/35	0.84	0.24	55,87,109,111	0
7	P6G	B	402	19/19	0.87	0.19	48,61,74,76	0
9	LMT	E	401	32/35	0.88	0.30	70,87,111,115	0
7	P6G	A	501	19/19	0.90	0.26	48,63,69,69	0
7	P6G	D	402	19/19	0.92	0.12	58,66,80,81	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 P6G E 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
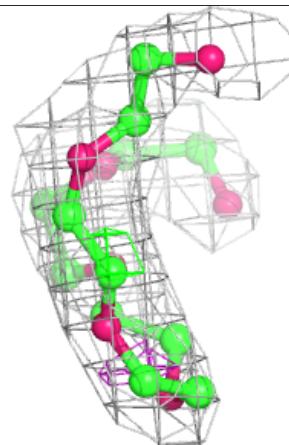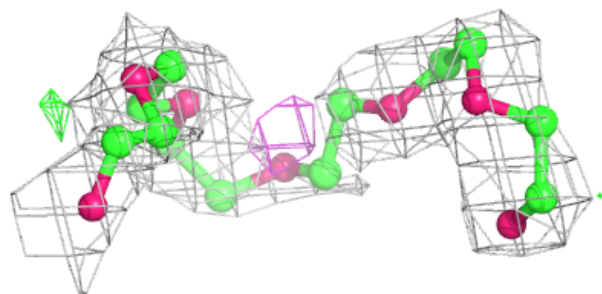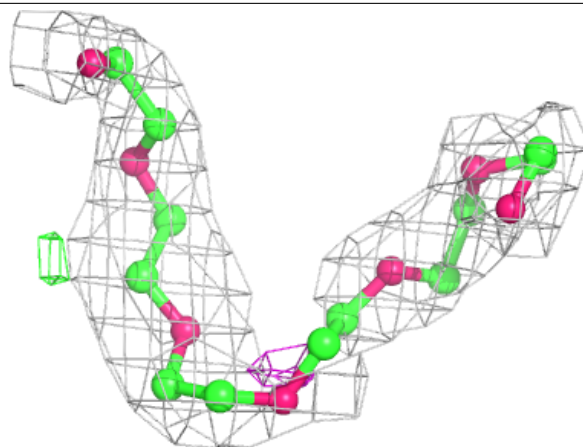
Electron density around PTY A 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
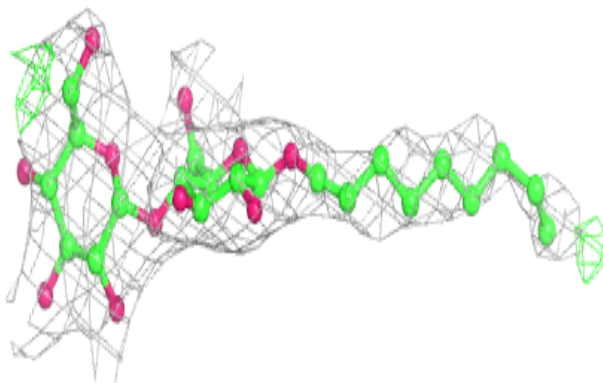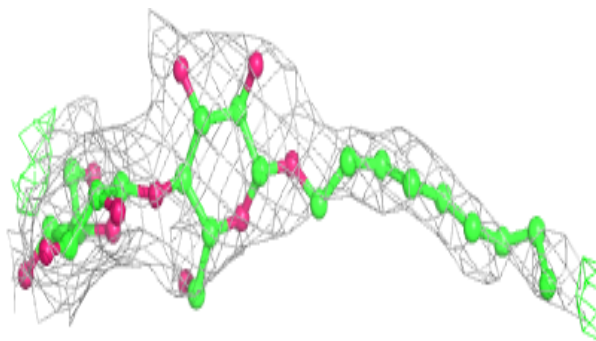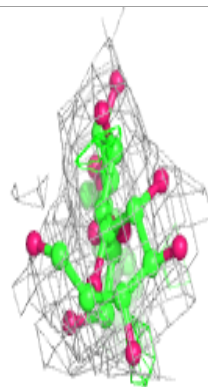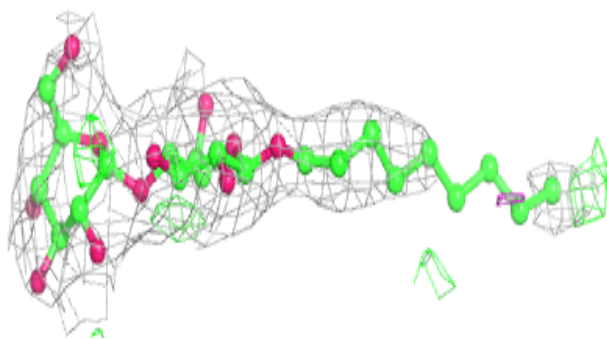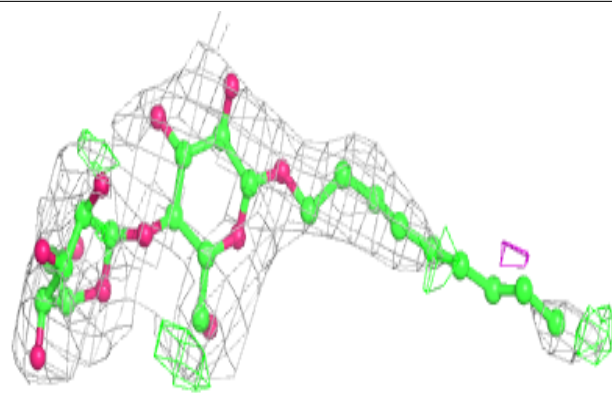$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
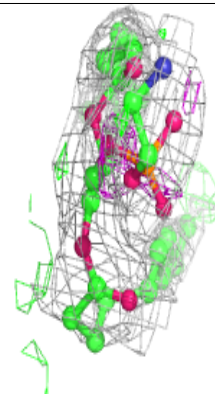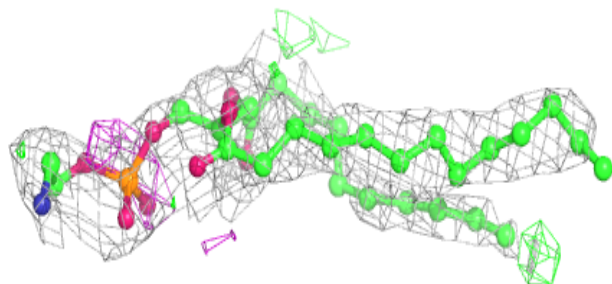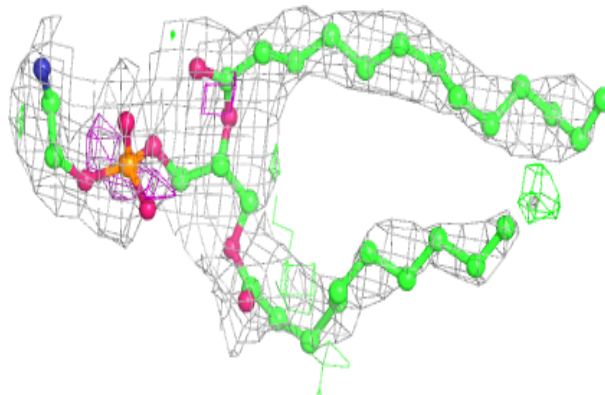
Electron density around LMT D 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
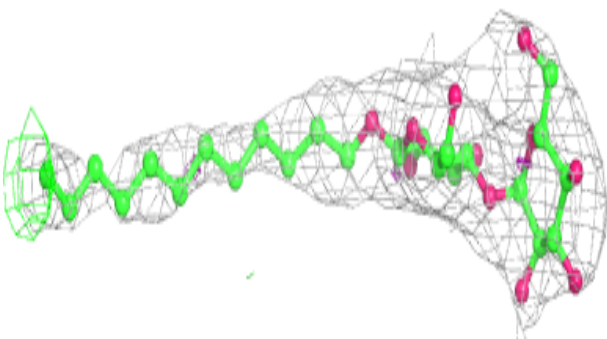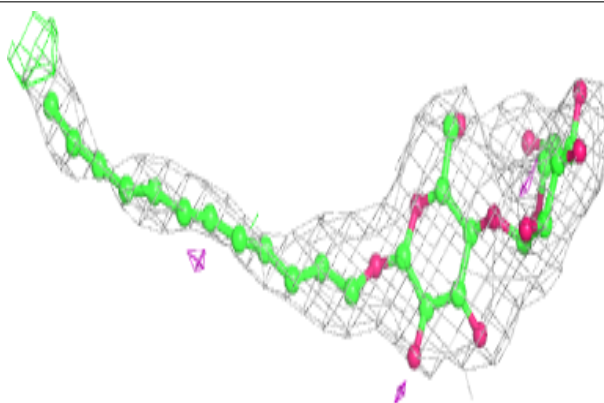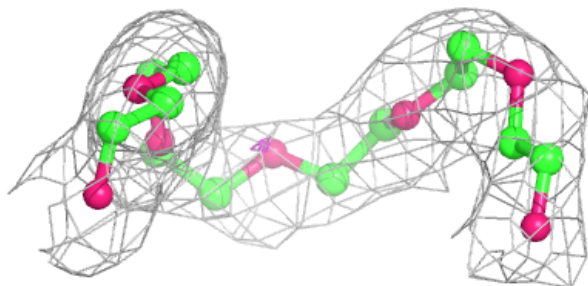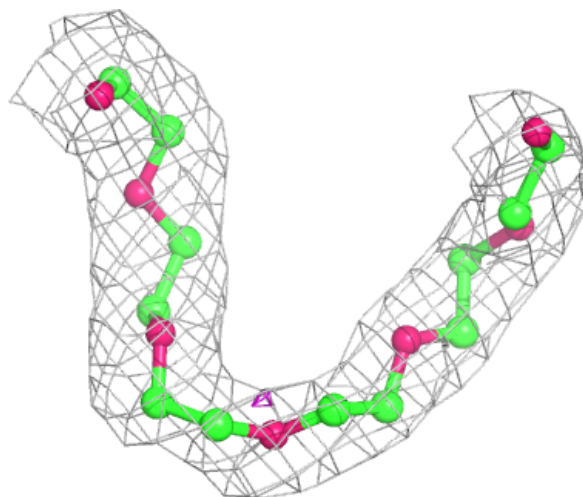mF_o-DF_c (at 3 rmsd) in purple (negative)
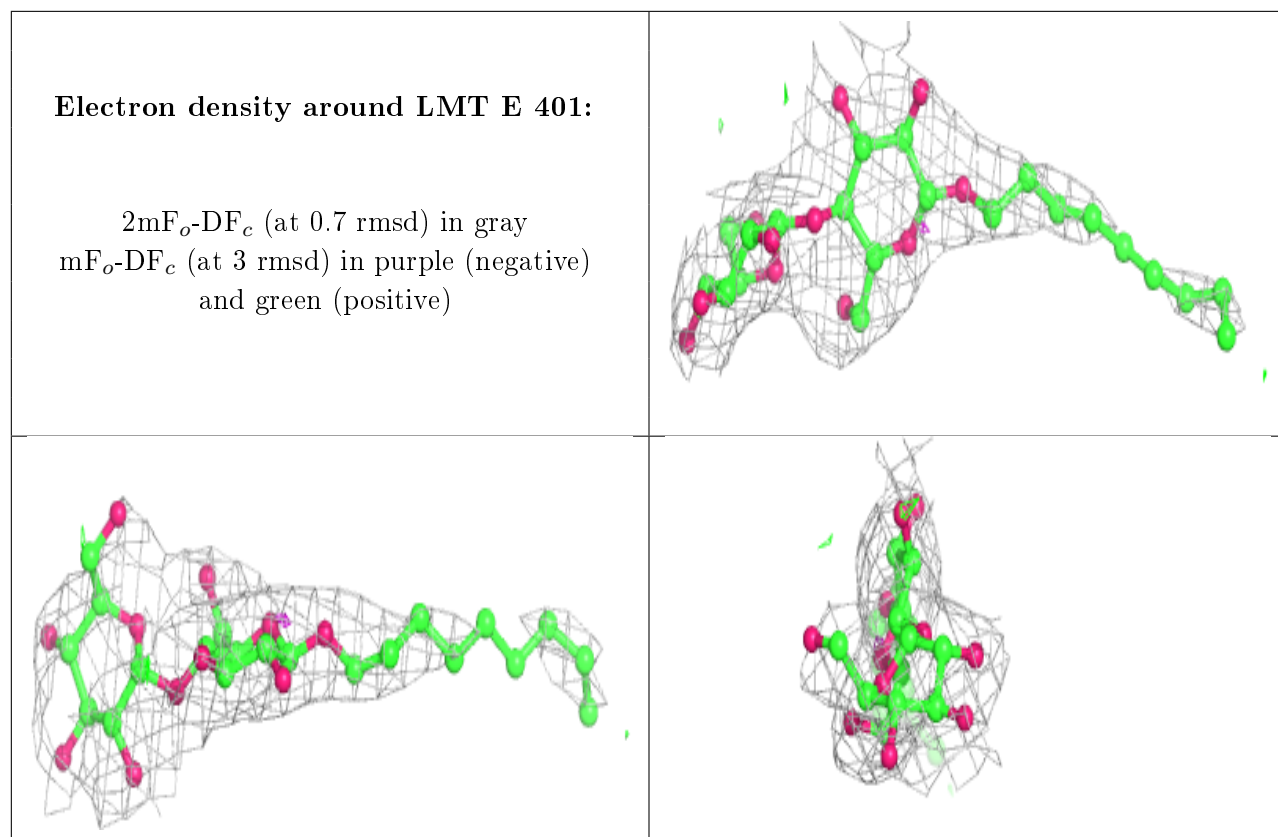and green (positive)
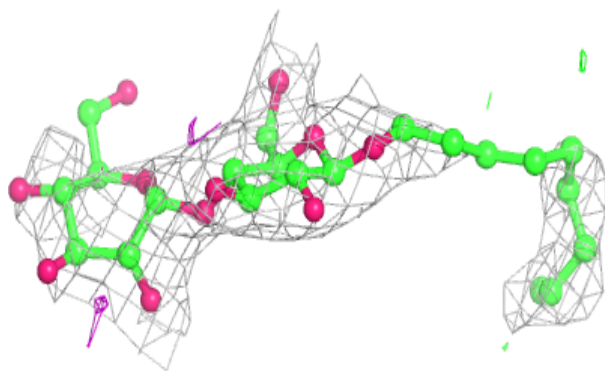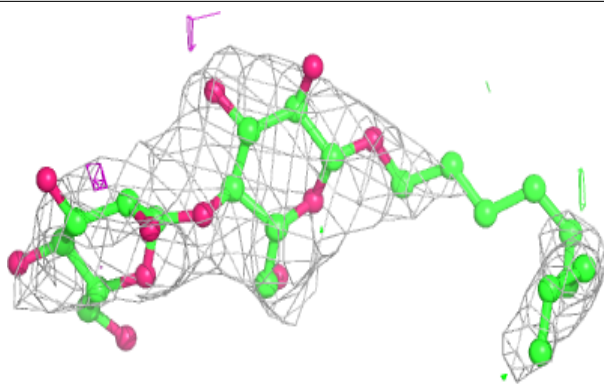
Electron density around LMT C 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
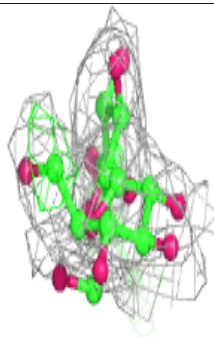
Electron density around LMT A 503:

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

Electron density around LMT B 401:

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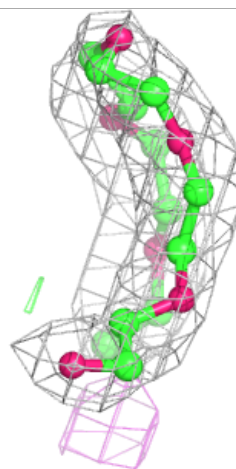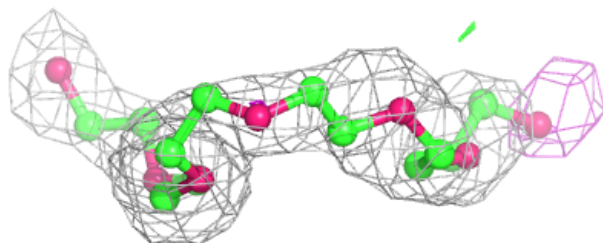and green (positive)

Electron density around P6G B 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
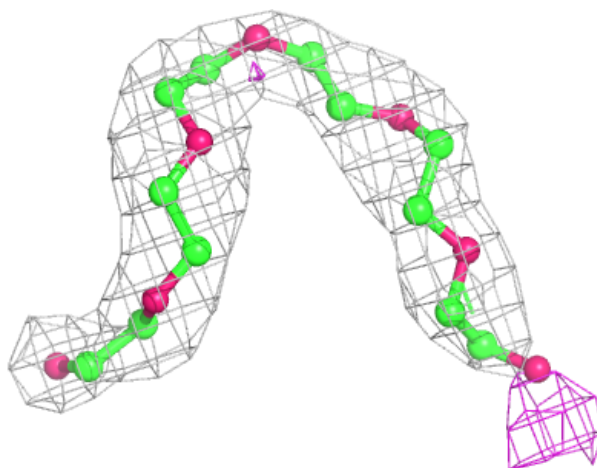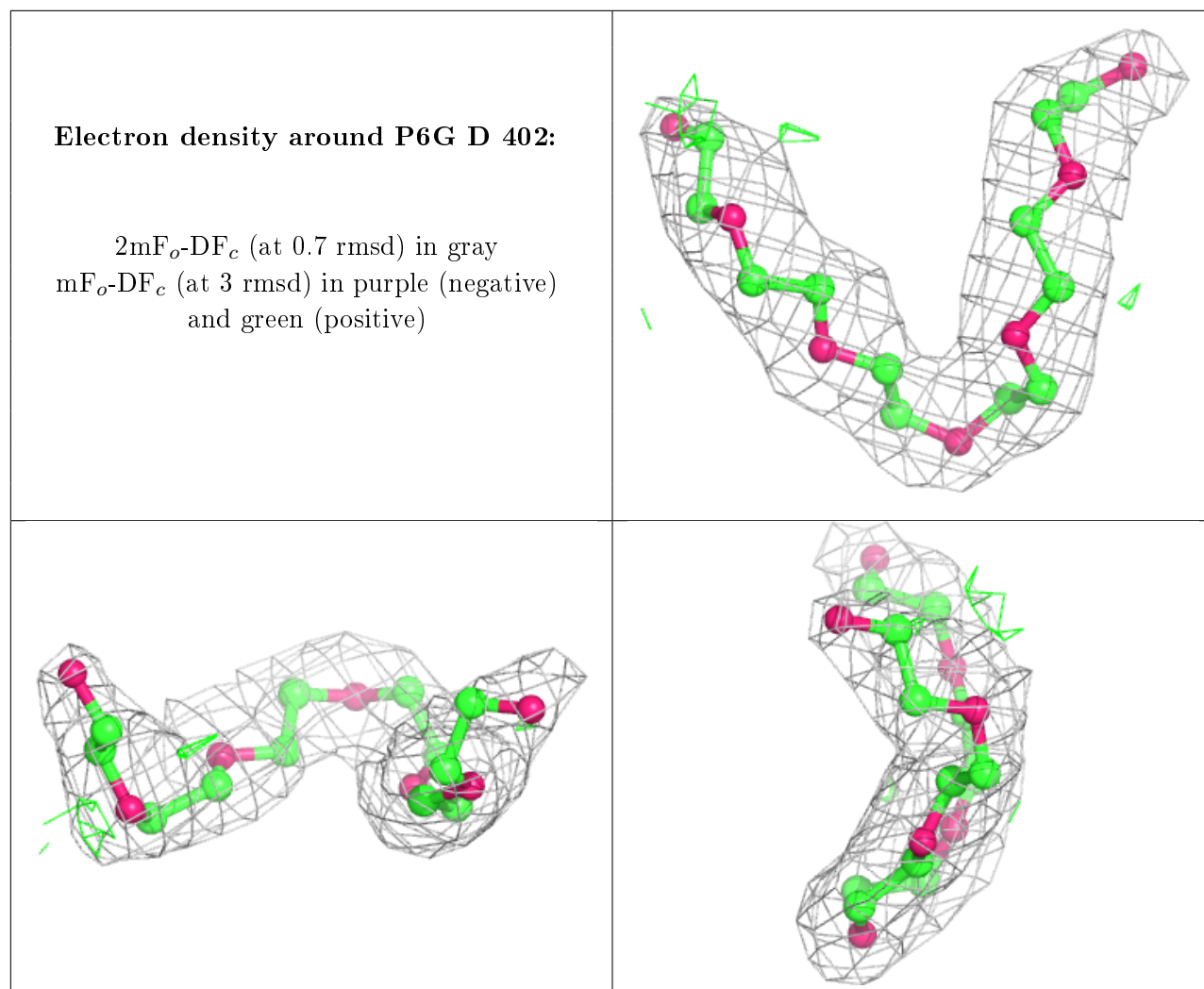
Electron density around LMT E 401:

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

Electron density around P6G A 501:

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

Electron density around P6G D 402:

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

6.5 Other polymers (i)

There are no such residues in this entry.