Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:06 am BST

PDB ID	:	4JAQ
Title	:	Crystal Structure of Mycobacterium tuberculosis PKS11 Reveals Intermediates in the Synthesis of Methyl-branched Alkylpyrones
Authors	:	Gokulan, K.; Sacchettini, J.C.; Mycobacterium Tuberculosis Structural Proteomics Project (XMTB)
Deposited on	:	2013-02-19
Resolution	:	1.73 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

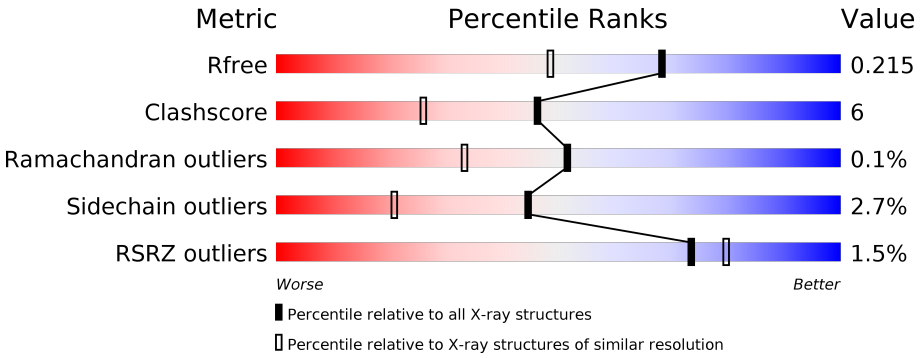
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.73 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	353	89% 10%
1	B	353	86% 13%
1	C	353	85% 14%
1	D	353	86% 13%

2 Entry composition

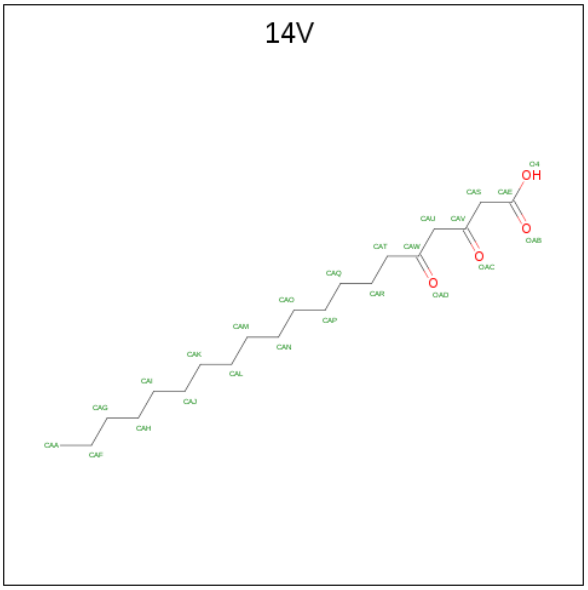
There are 5 unique types of molecules in this entry. The entry contains 11571 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-pyrone synthesis polyketide synthase-like Pks11.

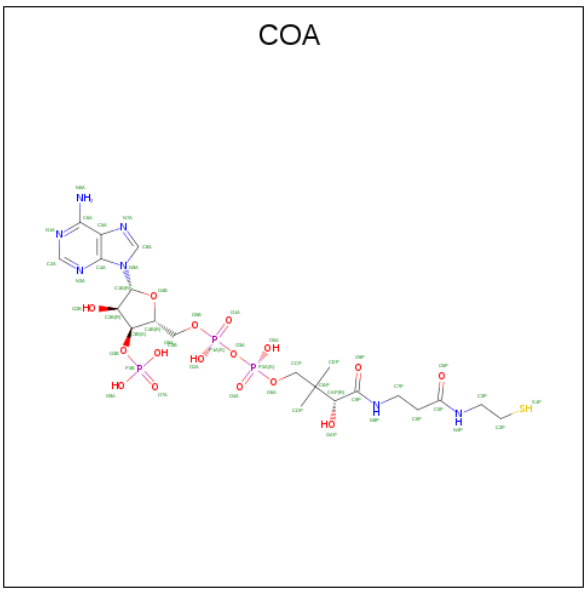
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	352	Total	C	N	O	S	0	0	0
			2642	1671	469	494	8			
1	A	352	Total	C	N	O	S	0	0	0
			2642	1671	469	494	8			
1	C	352	Total	C	N	O	S	0	0	0
			2642	1671	469	494	8			
1	B	352	Total	C	N	O	S	0	0	0
			2642	1671	469	494	8			

- Molecule 2 is 3,5-dioxoicosanoic acid (three-letter code: 14V) (formula: $C_{20}H_{36}O_4$).



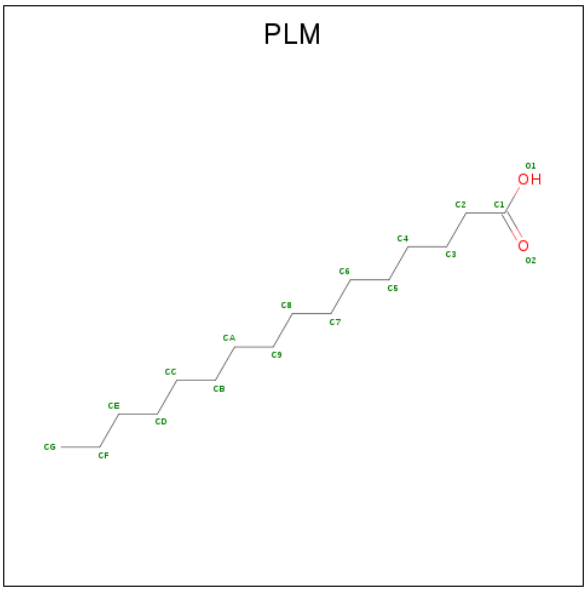
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	O		0	0
			23	20	3			
2	A	1	Total	C	O		0	0
			23	20	3			

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			17	16	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			18	16	2		

- Molecule 5 is water.

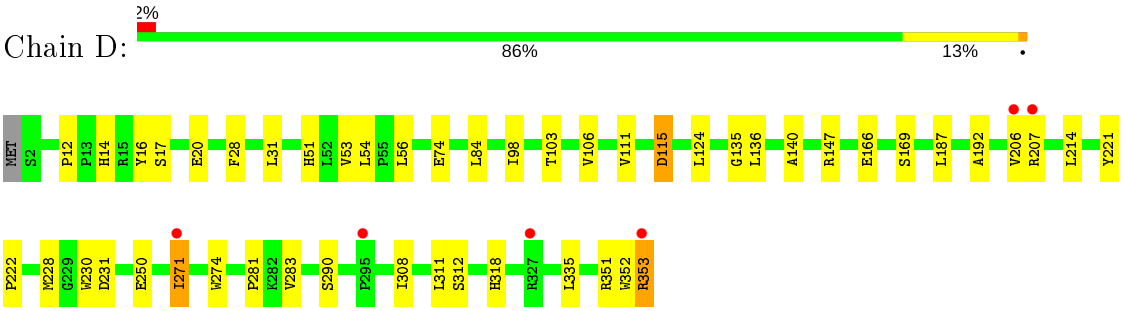
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	191	Total	O	0	0
			191	191		
5	A	198	Total	O	0	0
			198	198		
5	C	215	Total	O	0	0
			215	215		
5	B	222	Total	O	0	0
			222	222		

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.

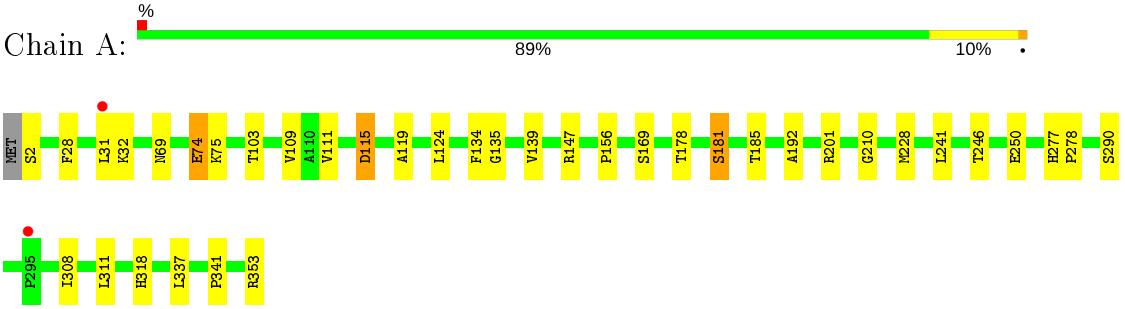
- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

Chain D:



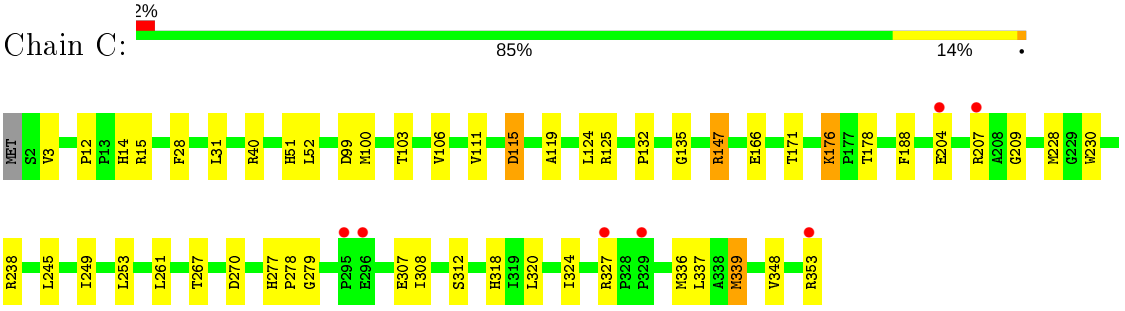
- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

Chain A:



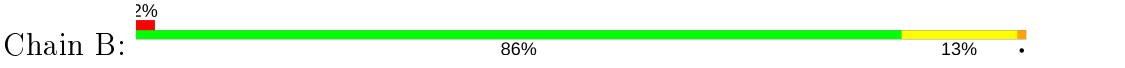
- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

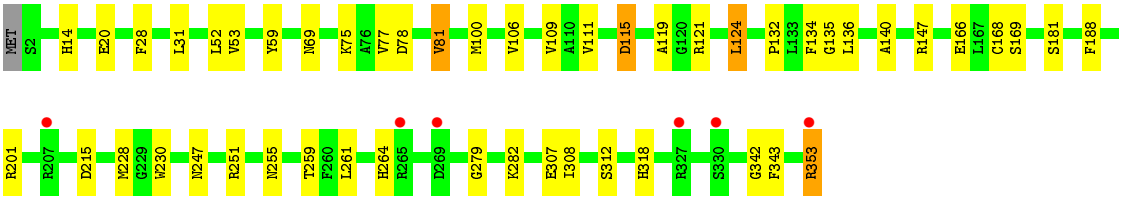
Chain C:



- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

Chain B:




MET
S2
H14
E20
F28
L31
L52
V53
Y59
N69
K75
A76
V77
D78
V81
M100
V106
V109
A110
V111
D115
A119
G120
R121
L124
P132
L133
F134
G135
L136
A140
R147
E166
L167
C168
S169
S181
F188
R201
R207
D215
M228
G229
W230
N247
R251
N255
T259
F260
L261
H264
R265
D269
G279
K282
E307
I308
S312
H318
R327
S330
G342
F343
R353

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.01Å 48.71Å 194.29Å 90.00° 97.89° 90.00°	Depositor
Resolution (Å)	48.11 – 1.73 48.11 – 1.73	Depositor EDS
% Data completeness (in resolution range)	89.7 (48.11-1.73) 89.7 (48.11-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 1.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.182 , 0.221 0.177 , 0.215	Depositor DCC
R_{free} test set	6346 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	17.5	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11571	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: 14V, COA, PLM

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	0.39	0/2695	0.54	0/3671
1	B	0.35	0/2695	0.55	0/3671
1	C	0.34	0/2695	0.54	0/3671
1	D	0.36	0/2695	0.54	0/3671
All	All	0.36	0/10780	0.54	0/14684

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	2642	0	2674	27	0
1	B	2642	0	2675	41	0
1	C	2642	0	2674	35	0
1	D	2642	0	2674	38	0
2	A	23	0	35	5	0
2	D	23	0	35	4	0
3	B	48	0	31	1	0
3	C	48	0	31	2	0
4	B	18	0	31	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	17	0	31	5	0
5	A	198	0	0	1	0
5	B	222	0	0	2	0
5	C	215	0	0	4	0
5	D	191	0	0	3	0
All	All	11571	0	10891	137	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 6.

All (137) 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:D:352:TRP:O	1:D:353:ARG:HG3	1.66	0.93
1:B:353:ARG:HH11	1:B:353:ARG:CG	1.83	0.91
1:B:119:ALA:HA	1:B:124:LEU:HG	1.53	0.91
1:A:69:ASN:HD21	1:A:109:VAL:H	1.18	0.88
1:B:353:ARG:HH11	1:B:353:ARG:HG2	1.38	0.88
1:B:69:ASN:HD21	1:B:109:VAL:H	1.17	0.85
1:B:247:ASN:HD21	1:B:251:ARG:HH21	1.19	0.85
1:C:209:GLY:O	1:C:353:ARG:HG3	1.81	0.81
1:A:119:ALA:HA	1:A:124:LEU:HG	1.64	0.79
1:C:119:ALA:HA	1:C:124:LEU:HG	1.65	0.78
1:B:247:ASN:ND2	1:B:251:ARG:HH21	1.82	0.77
1:A:178:THR:HG22	1:A:181:SER:HB2	1.69	0.74
1:D:353:ARG:O	1:D:353:ARG:HD2	1.87	0.74
1:B:28:PHE:HB2	1:B:31:LEU:HD12	1.70	0.73
1:C:15:ARG:HD2	1:C:51:HIS:CE1	2.25	0.72
1:C:28:PHE:HB2	1:C:31:LEU:HD12	1.70	0.71
1:D:318:HIS:HD2	5:D:665:HOH:O	1.73	0.70
2:D:401:14V:HAS	2:D:401:14V:HAR	1.73	0.69
1:B:255:ASN:O	1:B:259:THR:HG23	1.96	0.66
1:D:106:VAL:HG22	1:D:230:TRP:HE1	1.62	0.65
1:A:28:PHE:HB2	1:A:31:LEU:HD12	1.79	0.64
1:C:279:GLY:HA3	3:C:401:COA:H22	1.80	0.63
1:C:176:LYS:HE3	1:C:238:ARG:HD3	1.81	0.63
1:D:353:ARG:HD3	1:B:201:ARG:HD2	1.80	0.63
1:B:188:PHE:CD2	4:B:402:PLM:H52	2.34	0.62
2:A:401:14V:HAR	2:A:401:14V:HAS	1.81	0.62
1:A:178:THR:HG23	1:A:181:SER:H	1.65	0.62
1:B:188:PHE:CD1	4:B:402:PLM:H41	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:VAL:O	1:B:81:VAL:HG13	2.01	0.60
1:D:353:ARG:HD3	1:B:201:ARG:CD	2.31	0.60
1:C:40:ARG:HD2	5:C:625:HOH:O	2.02	0.59
1:C:307:GLU:HG3	1:C:308:ILE:HG23	1.85	0.59
1:D:53:VAL:HG13	1:D:54:LEU:HD13	1.84	0.59
1:A:169:SER:HA	2:A:401:14V:HAIA	1.84	0.59
1:D:106:VAL:HG22	1:D:230:TRP:NE1	2.17	0.59
1:D:12:PRO:O	1:D:51:HIS:HD2	1.86	0.59
1:C:176:LYS:HD3	1:C:178:THR:HG23	1.85	0.57
1:A:178:THR:CG2	1:A:181:SER:HB2	2.34	0.57
1:D:353:ARG:HD2	1:D:353:ARG:C	2.23	0.57
1:D:352:TRP:O	1:D:353:ARG:CG	2.48	0.57
1:A:210:GLY:HA3	1:A:353:ARG:HG3	1.86	0.57
1:B:318:HIS:HD2	5:B:671:HOH:O	1.87	0.56
1:C:267:THR:HG22	1:C:270:ASP:OD2	2.05	0.56
1:B:168:CYS:HB3	4:B:402:PLM:H51	1.87	0.56
1:B:353:ARG:HH11	1:B:353:ARG:HG3	1.71	0.55
1:D:250:GLU:HA	1:D:290:SER:OG	2.06	0.55
1:D:271:ILE:HD11	1:D:274:TRP:CD1	2.42	0.55
1:A:32:LYS:HG3	1:A:32:LYS:O	2.07	0.55
1:B:106:VAL:HG22	1:B:230:TRP:HE1	1.71	0.54
1:D:111:VAL:HG22	1:C:135:GLY:HA2	1.90	0.54
1:A:210:GLY:HA3	1:A:353:ARG:CG	2.37	0.53
1:D:353:ARG:HB2	1:B:201:ARG:HD2	1.90	0.53
1:B:353:ARG:NH1	1:B:353:ARG:CG	2.53	0.53
1:A:156:PRO:HG2	1:A:201:ARG:NH1	2.23	0.53
1:B:279:GLY:HA3	3:B:401:COA:H22	1.91	0.52
1:B:78:ASP:OD1	1:B:121:ARG:NH1	2.42	0.52
4:C:402:PLM:H32	5:C:715:HOH:O	2.07	0.52
1:B:59:TYR:CE2	1:B:169:SER:HB3	2.43	0.52
1:D:166:GLU:HG3	1:D:312:SER:HB3	1.92	0.52
1:B:106:VAL:HG22	1:B:230:TRP:NE1	2.25	0.52
1:B:188:PHE:CG	4:B:402:PLM:H41	2.44	0.51
1:A:246:THR:O	1:A:250:GLU:HG3	2.11	0.51
1:D:271:ILE:HD11	1:D:274:TRP:CG	2.45	0.51
1:D:308:ILE:HD12	1:D:311:LEU:HD11	1.94	0.50
1:D:136:LEU:HB2	1:D:140:ALA:HB2	1.94	0.50
1:B:307:GLU:HG3	1:B:308:ILE:HG23	1.93	0.50
1:D:103:THR:HG23	1:D:115:ASP:HB3	1.94	0.49
1:D:228:MET:HE2	2:D:401:14V:CAV	2.42	0.49
1:C:204:GLU:O	1:C:207:ARG:HD3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ASP:OD2	1:B:264:HIS:HE1	1.95	0.49
1:B:247:ASN:HD21	1:B:251:ARG:NH2	1.98	0.49
1:A:135:GLY:HA2	1:B:111:VAL:HG22	1.94	0.49
1:C:249:ILE:HD11	1:C:339:MET:SD	2.52	0.49
1:B:53:VAL:HG21	1:B:75:LYS:HG3	1.94	0.48
1:D:214:LEU:HD11	1:D:351:ARG:HB2	1.94	0.48
1:A:111:VAL:HG22	1:B:135:GLY:HA2	1.96	0.48
1:C:99:ASP:OD1	1:C:125:ARG:NH1	2.42	0.48
1:C:171:THR:OG1	4:C:402:PLM:HA2	2.14	0.47
1:C:320:LEU:O	1:C:324:ILE:HG13	2.13	0.47
2:A:401:14V:CAR	2:A:401:14V:HAS	2.45	0.47
1:A:341:PRO:HD3	2:A:401:14V:OAB	2.14	0.47
1:C:3:VAL:HG11	1:C:353:ARG:HH22	1.80	0.47
1:A:74:GLU:HG3	5:A:680:HOH:O	2.14	0.46
1:D:98:ILE:HD12	1:D:124:LEU:HD21	1.98	0.46
1:C:277:HIS:ND1	1:C:278:PRO:HD2	2.30	0.45
1:B:53:VAL:HG21	1:B:75:LYS:CG	2.46	0.45
1:C:147:ARG:HA	1:C:147:ARG:HD3	1.46	0.45
1:A:250:GLU:HA	1:A:290:SER:OG	2.17	0.45
1:D:14:HIS:HB3	1:D:16:TYR:CE2	2.52	0.45
1:D:353:ARG:HD3	1:B:201:ARG:NE	2.32	0.45
1:C:166:GLU:HG3	1:C:312:SER:HB3	1.98	0.45
1:D:206:VAL:HG22	1:D:207:ARG:H	1.82	0.45
1:B:353:ARG:HG2	1:B:353:ARG:NH1	2.16	0.44
1:C:106:VAL:HG22	1:C:230:TRP:HE1	1.82	0.44
1:A:185:THR:HA	2:A:401:14V:HAJA	1.98	0.44
1:C:318:HIS:HD2	5:C:706:HOH:O	1.99	0.44
1:A:308:ILE:HD12	1:A:311:LEU:HD22	1.99	0.44
1:C:115:ASP:OD1	1:C:132:PRO:HB3	2.17	0.43
1:C:336:MET:HB2	1:C:348:VAL:HB	1.99	0.43
1:D:169:SER:HA	2:D:401:14V:HAIA	2.00	0.43
1:D:274:TRP:CZ3	1:D:335:LEU:HD23	2.53	0.43
1:A:103:THR:HG23	1:A:115:ASP:HB3	2.00	0.43
1:A:134:PHE:HB3	1:B:134:PHE:HB3	2.00	0.43
3:C:401:COA:O9P	3:C:401:COA:H141	2.18	0.43
1:A:74:GLU:HG2	1:A:75:LYS:N	2.33	0.43
1:C:188:PHE:CZ	4:C:402:PLM:H61	2.54	0.43
1:C:253:LEU:HD21	1:C:337:LEU:HD11	2.01	0.43
1:A:277:HIS:ND1	1:A:278:PRO:HD2	2.34	0.43
1:B:14:HIS:HB2	1:B:52:LEU:O	2.19	0.42
1:C:14:HIS:HB2	1:C:52:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:PHE:HB2	1:D:31:LEU:HD12	2.02	0.42
1:D:56:LEU:HA	1:D:56:LEU:HD23	1.91	0.42
1:B:166:GLU:HG3	1:B:312:SER:HB3	2.02	0.42
1:B:20:GLU:HG2	5:B:681:HOH:O	2.19	0.42
1:B:136:LEU:HB2	1:B:140:ALA:HB2	2.01	0.42
1:C:147:ARG:HD2	5:C:642:HOH:O	2.18	0.42
1:A:156:PRO:HG2	1:A:201:ARG:CZ	2.50	0.42
1:B:115:ASP:OD1	1:B:132:PRO:HB3	2.19	0.42
1:B:342:GLY:N	1:B:343:PHE:HA	2.35	0.42
1:C:103:THR:HG23	1:C:115:ASP:HB3	2.00	0.42
1:C:245:LEU:C	1:C:245:LEU:HD23	2.39	0.42
1:C:12:PRO:O	1:C:51:HIS:HD2	2.03	0.42
1:A:337:LEU:C	1:A:337:LEU:HD23	2.41	0.41
1:D:192:ALA:O	1:D:318:HIS:HE1	2.02	0.41
1:C:228:MET:SD	4:C:402:PLM:O1	2.78	0.41
1:C:106:VAL:HG22	1:C:230:TRP:NE1	2.35	0.41
1:D:28:PHE:HE2	2:D:401:14V:CAA	2.33	0.41
1:A:228:MET:HG3	1:A:241:LEU:CD1	2.49	0.41
1:D:206:VAL:HG22	1:D:207:ARG:N	2.36	0.41
1:B:215:ASP:OD2	1:B:264:HIS:CE1	2.74	0.41
1:D:17:SER:OG	1:D:20:GLU:HG3	2.21	0.40
1:D:221:TYR:HA	1:D:222:PRO:HD3	1.90	0.40
1:A:192:ALA:O	1:A:318:HIS:HE1	2.04	0.40
1:D:135:GLY:HA2	1:C:111:VAL:HG22	2.02	0.40
1:C:188:PHE:CD2	4:C:402:PLM:H72	2.56	0.40
1:D:281:PRO:HD2	5:D:630:HOH:O	2.22	0.40
1:D:283:VAL:HG23	5:D:647:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	350/353 (99%)	342 (98%)	8 (2%)	0	100 100
1	B	350/353 (99%)	343 (98%)	7 (2%)	0	100 100
1	C	350/353 (99%)	342 (98%)	7 (2%)	1 (0%)	41 23
1	D	350/353 (99%)	339 (97%)	11 (3%)	0	100 100
All	All	1400/1412 (99%)	1366 (98%)	33 (2%)	1 (0%)	51 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	327	ARG

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	280/281 (100%)	274 (98%)	6 (2%)	53 30
1	B	280/281 (100%)	270 (96%)	10 (4%)	35 12
1	C	280/281 (100%)	274 (98%)	6 (2%)	53 30
1	D	280/281 (100%)	272 (97%)	8 (3%)	42 18
All	All	1120/1124 (100%)	1090 (97%)	30 (3%)	44 21

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	74	GLU
1	D	84	LEU
1	D	115	ASP
1	D	147	ARG
1	D	187	LEU
1	D	231	ASP
1	D	271	ILE
1	D	353	ARG
1	A	2	SER
1	A	74	GLU

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Mol	Chain	Res	Type
1	A	115	ASP
1	A	139	VAL
1	A	147	ARG
1	A	181	SER
1	C	100	MET
1	C	115	ASP
1	C	147	ARG
1	C	176	LYS
1	C	261	LEU
1	C	339	MET
1	B	81	VAL
1	B	100	MET
1	B	115	ASP
1	B	124	LEU
1	B	147	ARG
1	B	181	SER
1	B	228	MET
1	B	261	LEU
1	B	282	LYS
1	B	353	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	51	HIS
1	D	92	ASN
1	D	318	HIS
1	A	69	ASN
1	A	318	HIS
1	C	34	HIS
1	C	51	HIS
1	C	318	HIS
1	B	51	HIS
1	B	57	GLN
1	B	69	ASN
1	B	247	ASN
1	B	264	HIS
1	B	318	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	COA	C	401	-	41,50,50	1.99	10 (24%)	52,75,75	1.35	5 (9%)
4	PLM	B	402	-	14,17,17	0.39	0	13,17,17	1.67	4 (30%)
2	14V	D	401	1	21,22,23	0.55	0	21,23,25	1.55	5 (23%)
4	PLM	C	402	1	16,16,17	0.96	1 (6%)	15,15,17	1.40	2 (13%)
2	14V	A	401	1	21,22,23	0.63	0	21,23,25	1.53	4 (19%)
3	COA	B	401	-	41,50,50	1.95	9 (21%)	52,75,75	1.41	9 (17%)

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	COA	C	401	-	-	6/44/64/64	0/3/3/3
4	PLM	B	402	-	-	1/13/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	14V	D	401	1	-	4/21/22/23	-
4	PLM	C	402	1	-	1/14/14/15	-
2	14V	A	401	1	-	6/21/22/23	-
3	COA	B	401	-	-	10/44/64/64	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	COA	C9P-N8P	6.36	1.47	1.33
3	B	401	COA	C9P-N8P	6.29	1.47	1.33
3	C	401	COA	C5P-N4P	5.18	1.45	1.33
3	B	401	COA	C5P-N4P	5.12	1.45	1.33
3	B	401	COA	P2A-O4A	4.65	1.67	1.50
3	C	401	COA	P2A-O4A	4.62	1.67	1.50
4	C	402	PLM	O1-C1	-3.35	1.24	1.42
3	C	401	COA	C6A-N6A	3.31	1.46	1.34
3	C	401	COA	C2B-C1B	-3.23	1.48	1.53
3	B	401	COA	C6A-N6A	3.20	1.45	1.34
3	B	401	COA	C2B-C1B	-2.98	1.49	1.53
3	C	401	COA	O2B-C2B	-2.75	1.36	1.43
3	B	401	COA	C2A-N3A	2.68	1.36	1.32
3	B	401	COA	O2B-C2B	-2.65	1.36	1.43
3	C	401	COA	P2A-O5A	2.58	1.67	1.55
3	B	401	COA	P2A-O5A	2.54	1.67	1.55
3	C	401	COA	C2A-N3A	2.50	1.36	1.32
3	C	401	COA	P2A-O6A	2.22	1.68	1.59
3	B	401	COA	P2A-O6A	2.21	1.68	1.59
3	C	401	COA	OAP-CAP	-2.02	1.38	1.42

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401	COA	N3A-C2A-N1A	-5.72	119.74	128.68
3	C	401	COA	N3A-C2A-N1A	-5.42	120.21	128.68
2	A	401	14V	CAM-CAL-CAK	-3.34	97.45	114.42
4	C	402	PLM	C9-C8-C7	-3.27	97.82	114.42
2	D	401	14V	CAO-CAN-CAM	-3.25	97.93	114.42
4	B	402	PLM	C8-C7-C6	3.18	130.55	114.42
2	D	401	14V	CAR-CAT-CAW	-3.11	106.61	114.60
2	A	401	14V	CAO-CAN-CAM	-3.06	98.90	114.42
4	C	402	PLM	C8-C7-C6	2.98	129.55	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	14V	CAM-CAL-CAK	-2.97	99.33	114.42
2	A	401	14V	CAR-CAT-CAW	-2.95	107.01	114.60
4	B	402	PLM	C4-C3-C2	-2.93	102.35	113.76
3	B	401	COA	C6P-C5P-N4P	2.50	120.63	116.42
2	A	401	14V	CAK-CAJ-CAI	-2.49	101.80	114.42
3	B	401	COA	P2A-O3A-P1A	-2.35	124.76	132.83
3	B	401	COA	O5A-P2A-O6A	2.26	118.22	107.75
3	C	401	COA	O6A-P2A-O4A	2.23	117.78	109.07
2	D	401	14V	CAK-CAJ-CAI	-2.21	103.21	114.42
3	C	401	COA	C3P-N4P-C5P	-2.21	118.74	122.84
3	B	401	COA	O6A-P2A-O4A	2.21	117.69	109.07
2	D	401	14V	CAQ-CAP-CAO	-2.20	103.25	114.42
3	C	401	COA	C6P-C5P-N4P	2.18	120.09	116.42
3	B	401	COA	O5P-C5P-N4P	-2.16	118.94	123.01
3	B	401	COA	C3P-N4P-C5P	-2.14	118.86	122.84
4	B	402	PLM	C5-C4-C3	2.12	125.21	114.42
4	B	402	PLM	CC-CB-CA	-2.06	103.97	114.42
3	C	401	COA	O5A-P2A-O6A	2.05	117.26	107.75
3	B	401	COA	C7P-C6P-C5P	-2.02	108.99	112.36
3	B	401	COA	O6A-CCP-CBP	-2.02	107.30	110.55

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	401	COA	C3B-O3B-P3B-O7A
3	C	401	COA	C5P-C6P-C7P-N8P
2	A	401	14V	CAW-CAU-CAV-CAS
2	A	401	14V	CAV-CAU-CAW-OAD
3	B	401	COA	C5B-O5B-P1A-O1A
3	B	401	COA	CCP-O6A-P2A-O5A
3	B	401	COA	CDP-CBP-CCP-O6A
3	B	401	COA	CAP-CBP-CCP-O6A
3	B	401	COA	CEP-CBP-CCP-O6A
3	B	401	COA	C2B-C3B-O3B-P3B
3	B	401	COA	C4B-C3B-O3B-P3B
2	A	401	14V	CAW-CAU-CAV-OAC
3	B	401	COA	C5P-C6P-C7P-N8P
3	C	401	COA	C3B-O3B-P3B-O9A
3	B	401	COA	C5B-O5B-P1A-O3A
3	B	401	COA	CCP-O6A-P2A-O3A
2	A	401	14V	CAR-CAT-CAW-CAU

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Mol	Chain	Res	Type	Atoms
2	A	401	14V	CAE-CAS-CAV-CAU
4	C	402	PLM	O1-C1-C2-C3
2	D	401	14V	CAR-CAT-CAW-CAU
3	C	401	COA	N8P-C9P-CAP-CBP
2	A	401	14V	CAR-CAT-CAW-OAD
2	D	401	14V	CAR-CAT-CAW-OAD
2	D	401	14V	CAE-CAS-CAV-CAU
4	B	402	PLM	C5-C6-C7-C8
2	D	401	14V	CAW-CAU-CAV-CAS
3	C	401	COA	C5B-O5B-P1A-O1A
3	C	401	COA	O9P-C9P-CAP-CBP

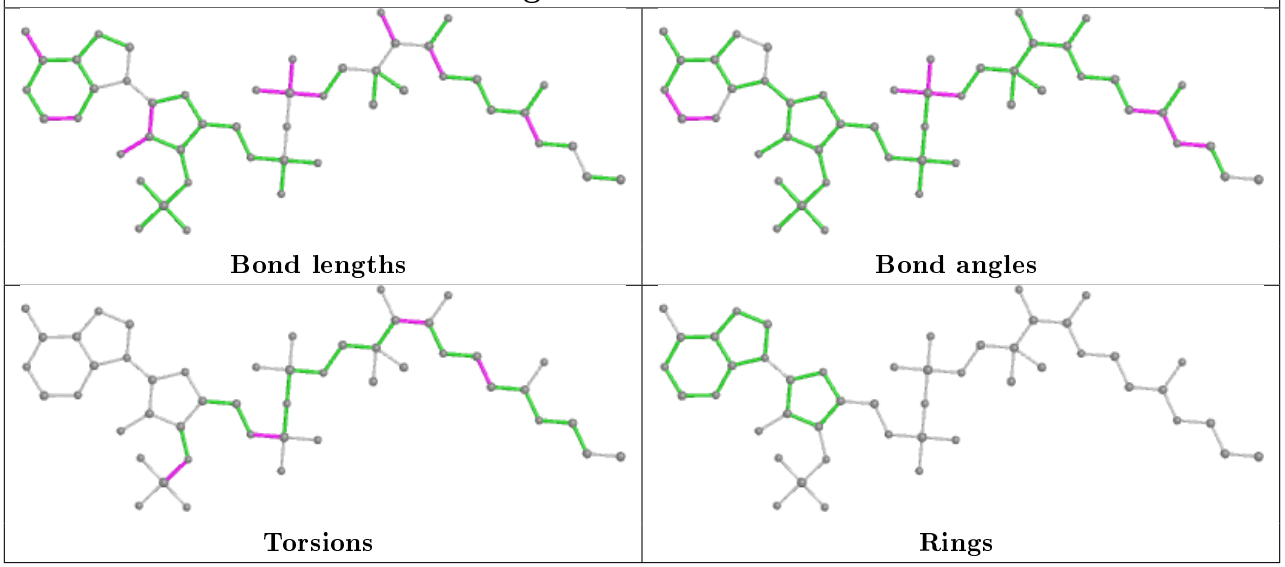
There are no ring outliers.

6 monomers are involved in 21 short contacts:

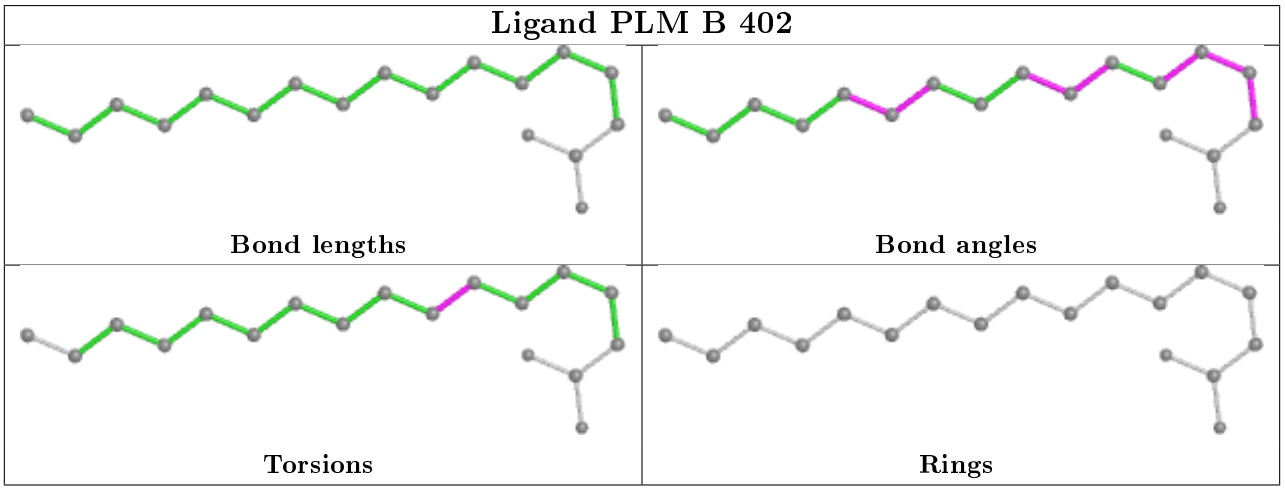
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	COA	2	0
4	B	402	PLM	4	0
2	D	401	14V	4	0
4	C	402	PLM	5	0
2	A	401	14V	5	0
3	B	401	COA	1	0

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.

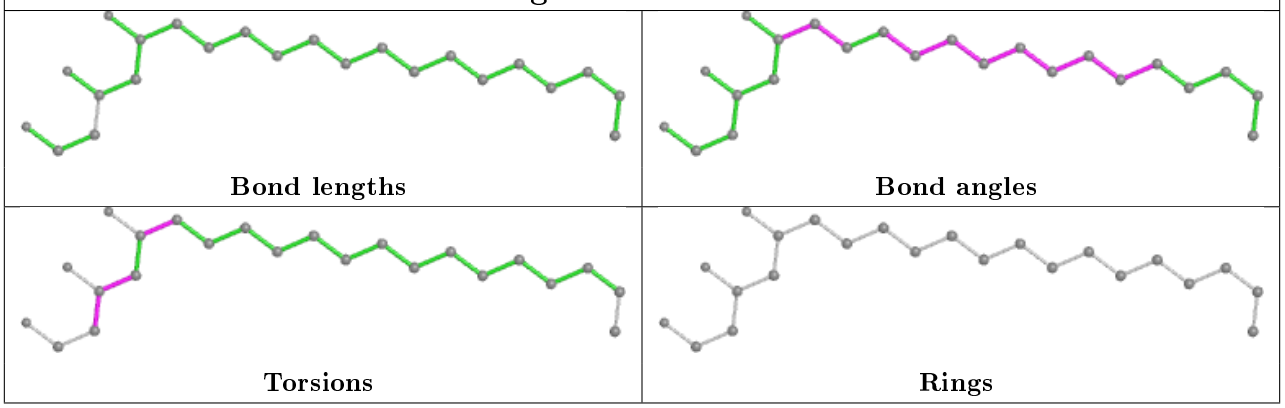
Ligand COA C 401

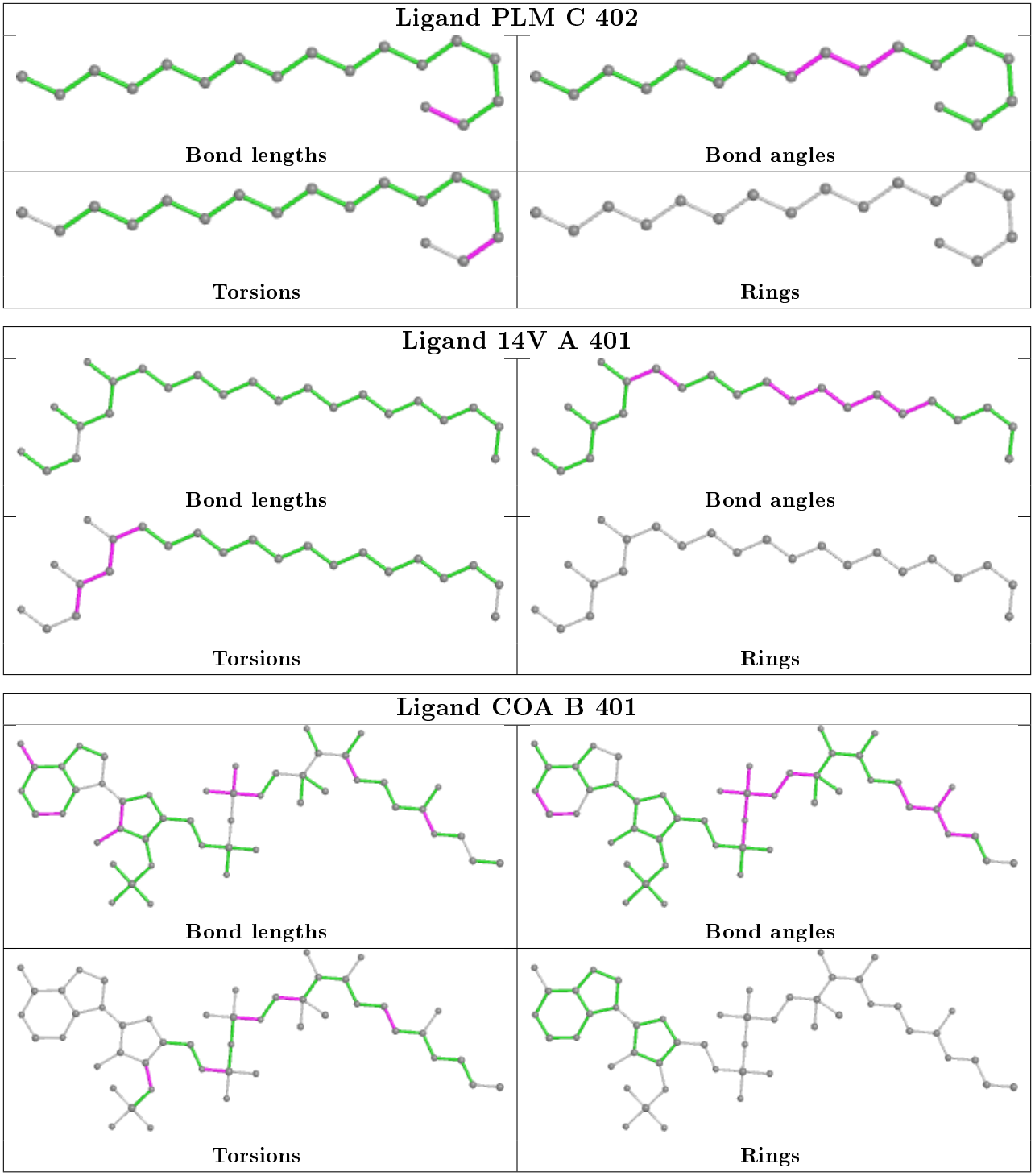


Ligand PLM B 402



Ligand 14V D 401





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	352/353 (99%)	-0.23	2 (0%) 89 92	9, 16, 30, 42	0
1	B	352/353 (99%)	-0.18	6 (1%) 70 76	9, 16, 30, 47	0
1	C	352/353 (99%)	-0.11	7 (1%) 65 71	9, 16, 31, 49	0
1	D	352/353 (99%)	-0.18	6 (1%) 70 76	9, 17, 32, 45	0
All	All	1408/1412 (99%)	-0.18	21 (1%) 73 80	9, 16, 31, 49	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	295	PRO	5.0
1	D	353	ARG	4.8
1	C	207	ARG	3.7
1	D	271	ILE	3.6
1	C	327	ARG	3.3
1	D	327	ARG	3.2
1	B	327	ARG	2.9
1	C	353	ARG	2.9
1	A	295	PRO	2.9
1	C	296	GLU	2.9
1	D	295	PRO	2.8
1	D	207	ARG	2.7
1	B	353	ARG	2.6
1	B	269	ASP	2.4
1	C	204	GLU	2.3
1	B	207	ARG	2.3
1	B	265	ARG	2.2
1	B	330	SER	2.1
1	D	206	VAL	2.1
1	A	31	LEU	2.0
1	C	329	PRO	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)

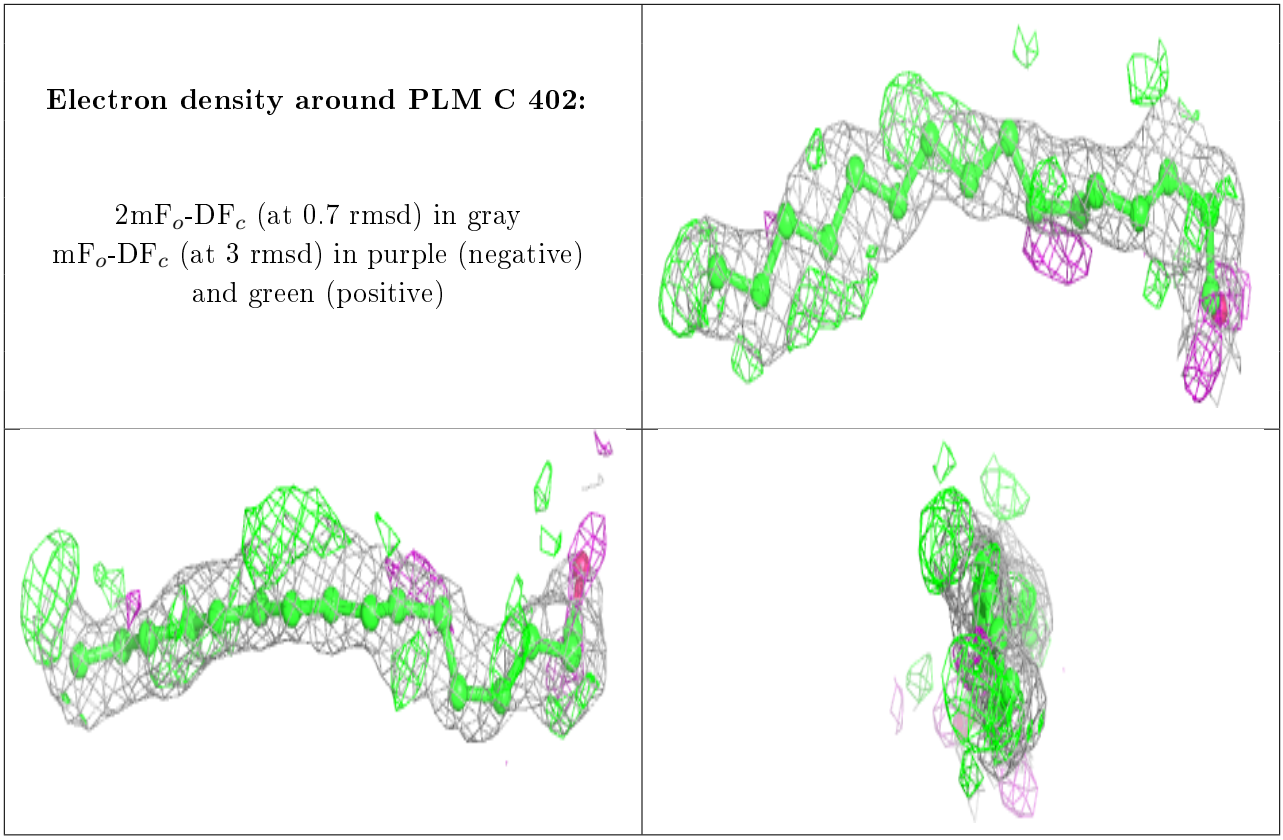
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	PLM	C	402	17/18	0.71	0.20	19,26,31,37	0
2	14V	D	401	23/24	0.78	0.19	20,27,34,35	0
4	PLM	B	402	18/18	0.78	0.21	17,25,38,40	0
2	14V	A	401	23/24	0.78	0.20	20,27,36,37	0
3	COA	C	401	48/48	0.84	0.22	24,37,54,63	0
3	COA	B	401	48/48	0.84	0.21	24,37,50,56	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.

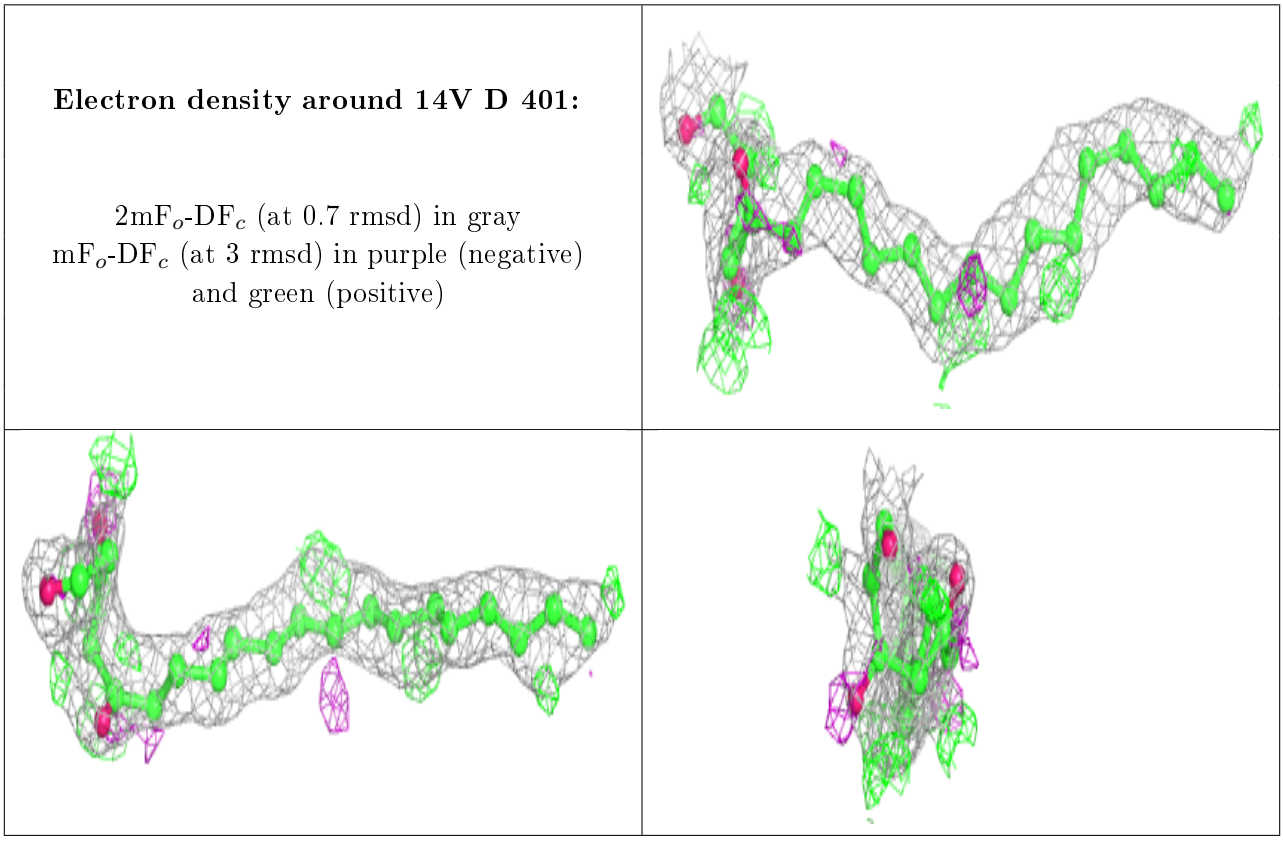
Electron density around PLM C 402:

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



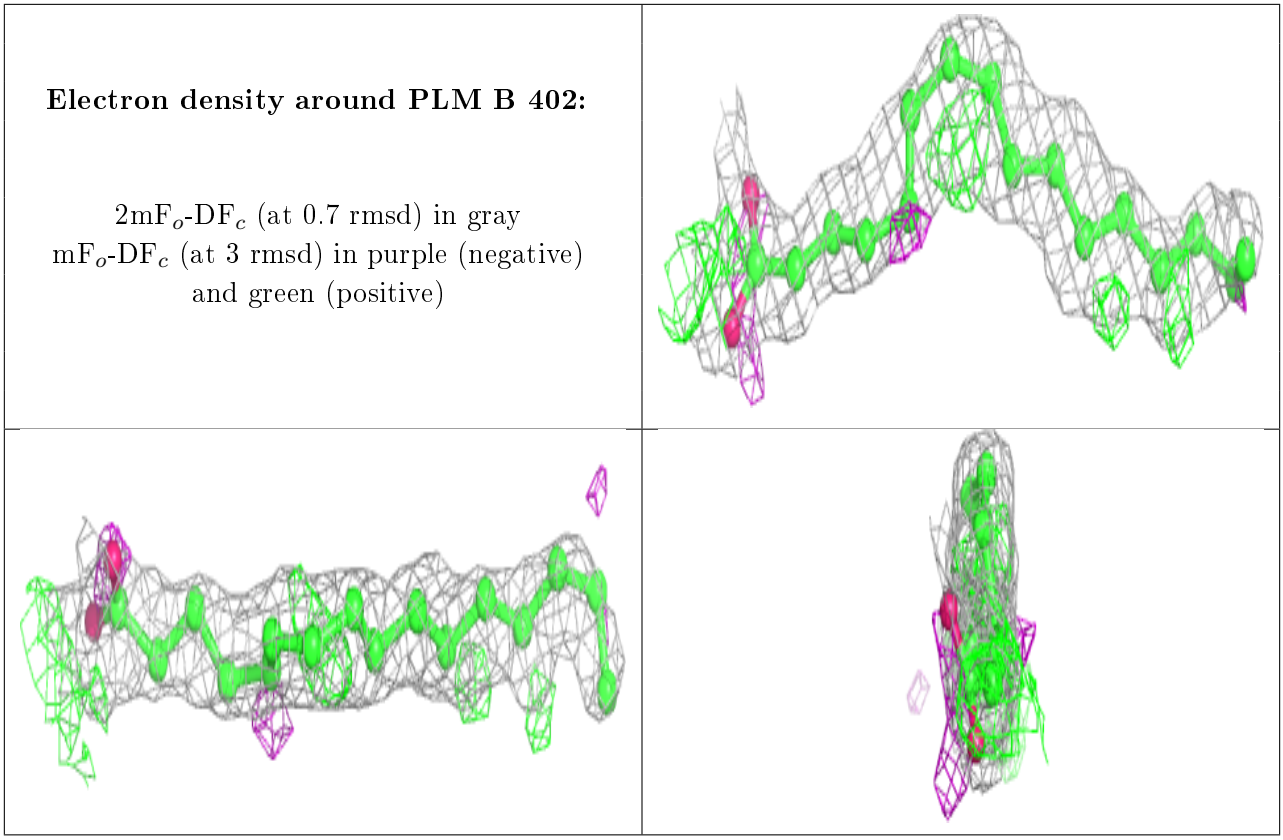
Electron density around 14V D 401:

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



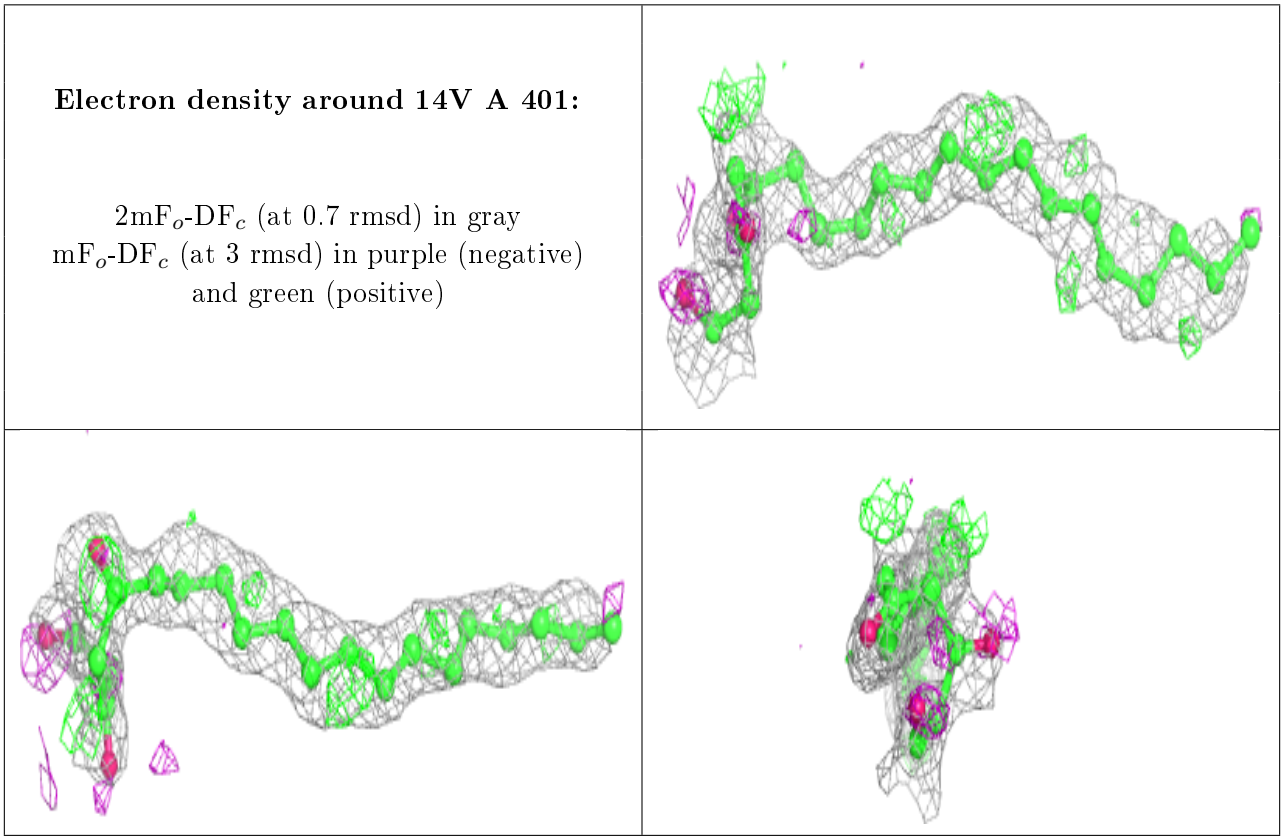
Electron density around PLM B 402:

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



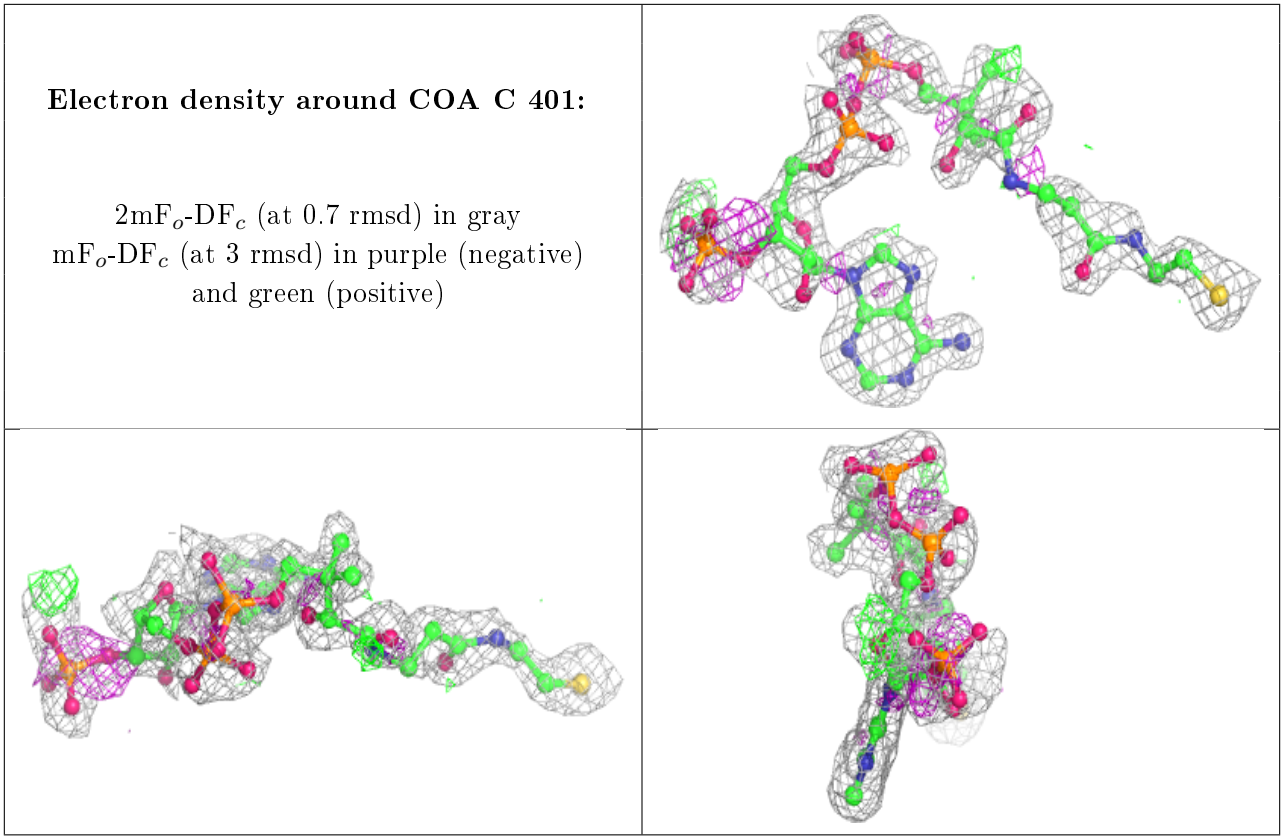
Electron density around 14V A 401:

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



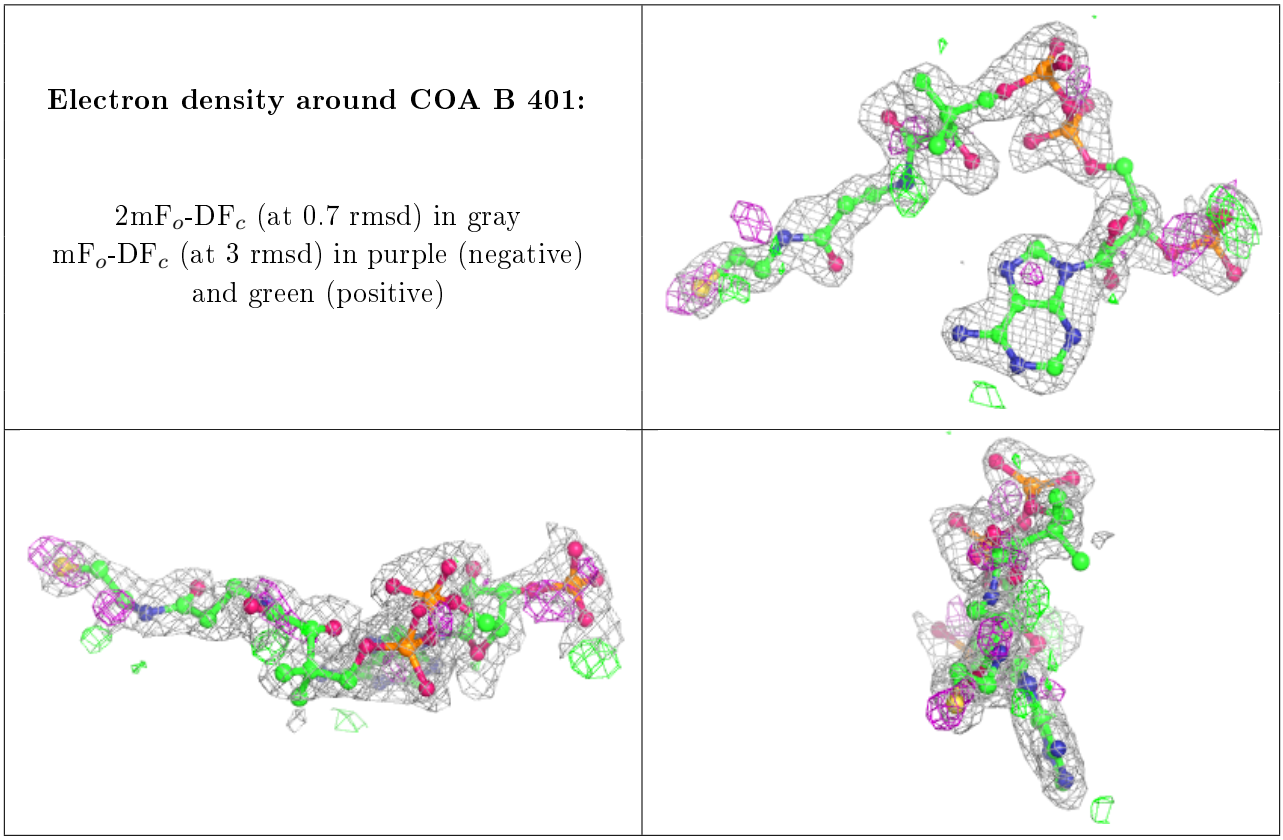
Electron density around COA C 401:

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



Electron density around COA 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)



6.5 Other polymers (i)

There are no such residues in this entry.