



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:27 pm BST

PDB ID : 4JAP
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 : 1.83 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

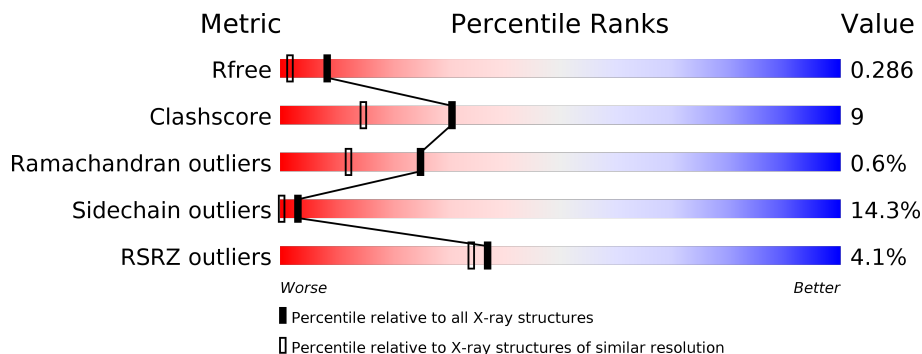
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	353	
1	B	353	
1	C	353	
1	D	353	

2 Entry composition [i](#)

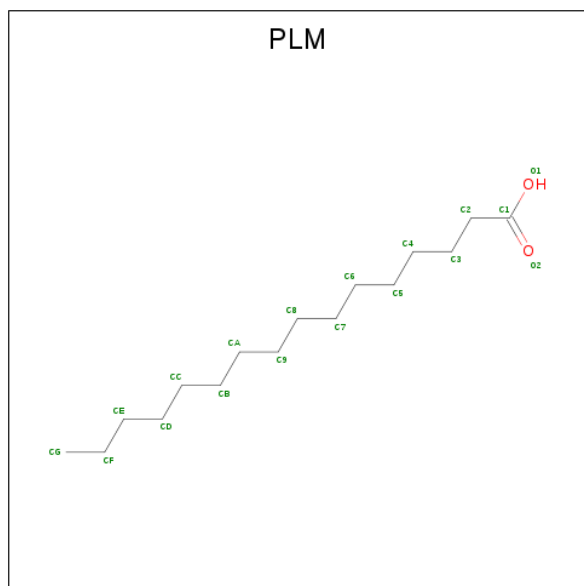
There are 5 unique types of molecules in this entry. The entry contains 10941 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

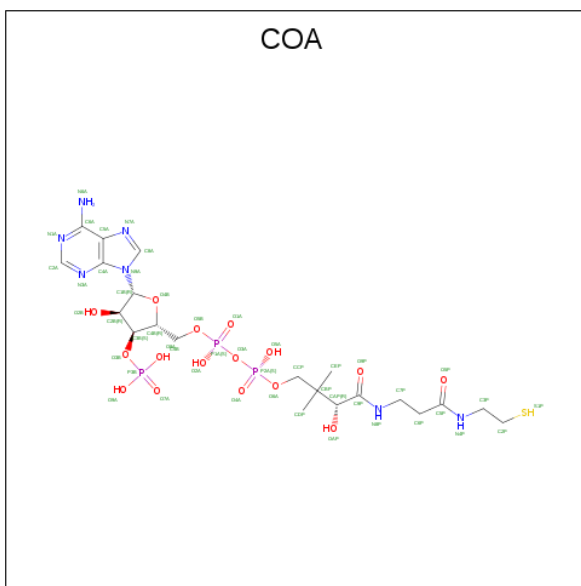
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	352	Total 2642	C 1671	N 469	O 494	S 8	0	0	0
1	C	353	Total 2649	C 1676	N 470	O 494	S 9	0	0	0
1	B	352	Total 2641	C 1671	N 469	O 493	S 8	0	0	0
1	A	353	Total 2650	C 1676	N 470	O 495	S 9	0	0	0

- Molecule 2 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



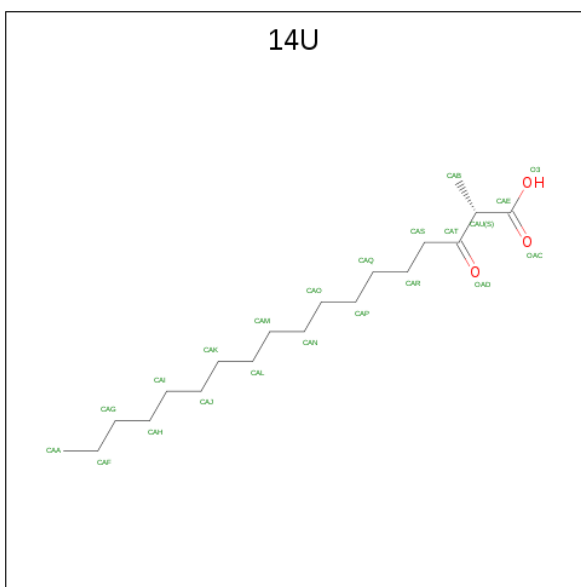
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	D	1	Total 18	C 16	O 2	0	0
2	C	1	Total 18	C 16	O 2	0	0

- 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	
			Total	C	N	O	P			S
3	C	1	48	21	7	16	3	1	0	0
3	B	1	48	21	7	16	3	1	0	0

- Molecule 4 is (2S)-2-methyl-3-oxooctadecanoic acid (three-letter code: 14U) (formula: $C_{19}H_{36}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			21	19	2		
4	A	1	Total	C	O	0	0
			21	19	2		

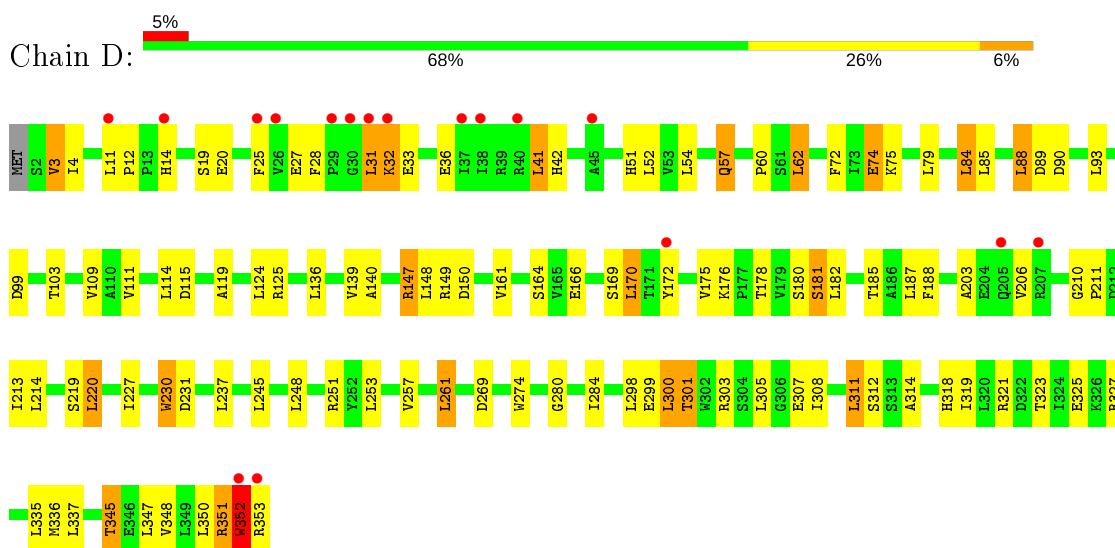
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	32	Total	O	0	0
			32	32		
5	C	19	Total	O	0	0
			19	19		
5	B	83	Total	O	0	0
			83	83		
5	A	51	Total	O	0	0
			51	51		

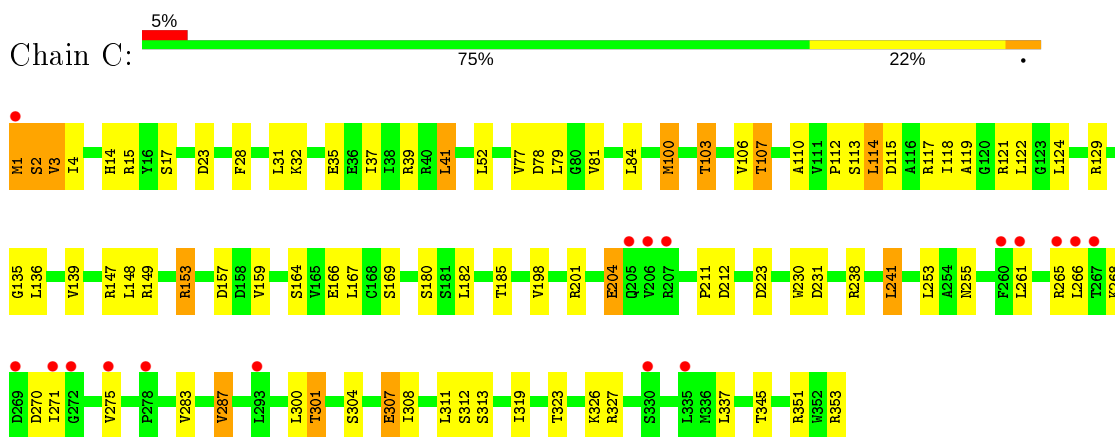
3 Residue-property plots [i](#)

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.

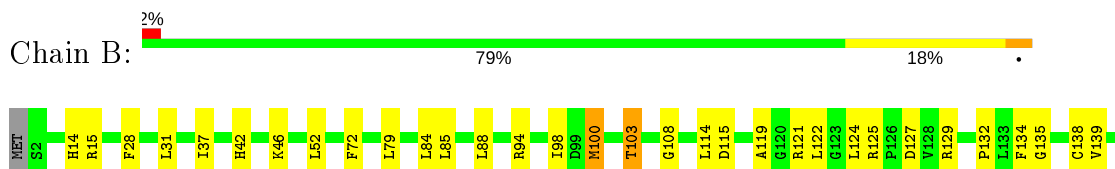
- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

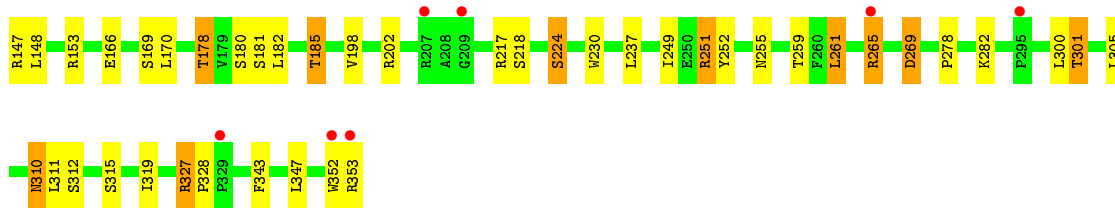


- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

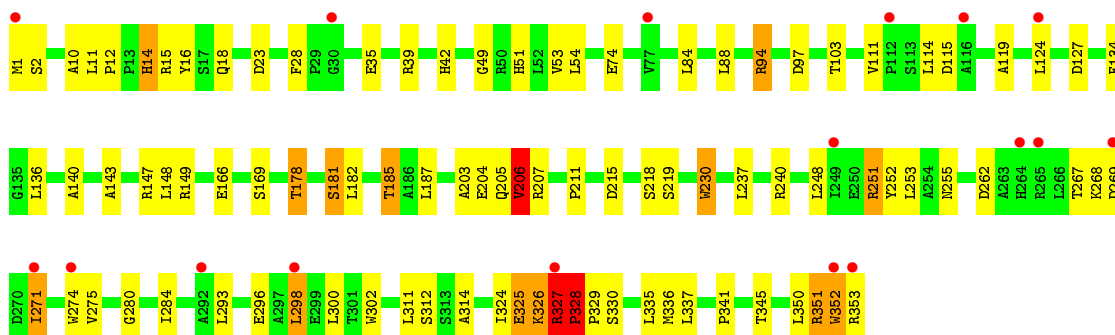
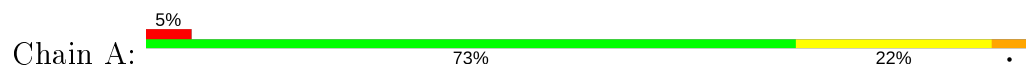


- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.01Å 48.63Å 193.66Å 90.00° 97.57° 90.00°	Depositor
Resolution (Å)	44.80 – 1.83 44.80 – 1.83	Depositor EDS
% Data completeness (in resolution range)	77.4 (44.80-1.83) 77.1 (44.80-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.83Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.234 , 0.289 0.230 , 0.286	Depositor DCC
R_{free} test set	4557 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtrriage
Anisotropy	0.093	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10941	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: COA, PLM, 14U

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	0.54	1/2703 (0.0%)	0.66	1/3681 (0.0%)
1	B	0.53	0/2694	0.65	0/3671
1	C	0.49	0/2702	0.57	0/3681
1	D	0.52	2/2695 (0.1%)	0.70	3/3671 (0.1%)
All	All	0.52	3/10794 (0.0%)	0.65	4/14704 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	351	ARG	C-N	8.77	1.54	1.34
1	D	352	TRP	C-N	-5.70	1.21	1.34
1	A	328	PRO	N-CD	5.22	1.55	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	352	TRP	O-C-N	-16.86	95.72	122.70
1	D	352	TRP	CA-C-N	9.46	138.01	117.20
1	D	351	ARG	C-N-CA	-8.57	100.27	121.70
1	A	327	ARG	C-N-CD	5.71	140.40	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	351	ARG	Mainchain
1	D	352	TRP	Mainchain

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	2650	0	2686	61	0
1	B	2641	0	2674	38	0
1	C	2649	0	2687	53	0
1	D	2642	0	2674	55	0
2	C	18	0	31	5	0
2	D	18	0	31	5	0
3	B	48	0	32	1	0
3	C	48	0	32	1	0
4	A	21	0	35	6	0
4	B	21	0	35	3	0
5	A	51	0	0	3	0
5	B	83	0	0	2	0
5	C	19	0	0	1	0
5	D	32	0	0	0	0
All	All	10941	0	10917	200	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 9.

All (200) 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:C:28:PHE:HB2	1:C:31:LEU:HD12	1.34	1.09
1:A:351:ARG:HG2	1:A:351:ARG:HH21	1.24	1.01
1:A:352:TRP:O	1:A:353:ARG:HB2	1.60	1.01
1:A:352:TRP:O	1:A:353:ARG:CB	2.18	0.92
1:C:23:ASP:OD1	1:C:39:ARG:NH2	2.04	0.91
1:C:107:THR:HG21	1:C:167:LEU:H	1.33	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ARG:HG2	1:B:252:TYR:CE1	2.07	0.90
1:B:224:SER:HB3	1:B:343:PHE:H	1.42	0.85
1:C:28:PHE:CB	1:C:31:LEU:HD12	2.05	0.85
1:C:1:MET:H2	1:C:149:ARG:HG3	1.42	0.83
1:B:28:PHE:HB2	1:B:31:LEU:HD12	1.64	0.80
1:D:219:SER:HB3	1:D:345:THR:HG22	1.62	0.79
1:C:28:PHE:HB2	1:C:31:LEU:CD1	2.14	0.75
1:C:1:MET:N	1:C:149:ARG:HG3	2.01	0.73
1:B:169:SER:HA	4:B:401:14U:HAK	1.71	0.72
1:A:18:GLN:N	5:A:523:HOH:O	2.22	0.72
1:A:328:PRO:HG3	1:A:352:TRP:CD2	2.27	0.70
1:C:107:THR:HG21	1:C:167:LEU:N	2.07	0.69
1:D:166:GLU:HG3	1:D:312:SER:HB3	1.76	0.66
1:C:169:SER:HA	2:C:401:PLM:HA2	1.77	0.65
1:D:169:SER:HA	2:D:401:PLM:HB1	1.79	0.65
1:A:166:GLU:HG3	1:A:312:SER:HB3	1.79	0.65
1:D:28:PHE:HB2	1:D:31:LEU:CD1	2.27	0.65
1:D:103:THR:HG21	1:D:114:LEU:HB2	1.79	0.64
1:A:178:THR:HG22	1:A:181:SER:H	1.62	0.64
1:D:188:PHE:CD2	2:D:401:PLM:H62	2.32	0.64
1:B:327:ARG:HG3	1:B:327:ARG:HH21	1.62	0.64
1:A:311:LEU:HB3	1:A:314:ALA:HB3	1.79	0.63
1:D:230:TRP:HH2	2:D:401:PLM:H52	1.62	0.63
1:C:119:ALA:HA	1:C:124:LEU:HG	1.80	0.63
1:B:178:THR:HG22	1:B:181:SER:H	1.64	0.62
1:C:301:THR:HB	1:C:319:ILE:HD13	1.81	0.62
1:A:219:SER:HB3	1:A:345:THR:HG22	1.82	0.62
1:D:84:LEU:HD22	1:D:88:LEU:HD22	1.81	0.62
1:A:169:SER:HA	4:A:401:14U:HAJA	1.81	0.61
1:D:4:ILE:HB	1:D:211:PRO:HD2	1.82	0.60
1:D:25:PHE:O	1:D:31:LEU:HD12	2.01	0.60
1:A:351:ARG:CG	1:A:351:ARG:HH21	2.07	0.60
1:B:119:ALA:HA	1:B:124:LEU:HG	1.82	0.60
1:D:28:PHE:HB2	1:D:31:LEU:HD12	1.84	0.59
1:A:185:THR:HA	4:A:401:14U:HAKA	1.84	0.59
1:A:352:TRP:O	1:A:353:ARG:CG	2.50	0.59
1:A:182:LEU:O	1:A:185:THR:HG22	2.03	0.59
1:D:300:LEU:HD23	1:D:323:THR:HG22	1.84	0.58
1:A:251:ARG:HB3	1:A:252:TYR:HD1	1.68	0.58
1:A:352:TRP:O	1:A:353:ARG:HG3	2.02	0.58
1:A:119:ALA:HA	1:A:124:LEU:HG	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ARG:HD3	5:B:534:HOH:O	2.04	0.58
1:A:351:ARG:NH2	1:A:351:ARG:HG2	2.03	0.58
1:A:324:ILE:HG12	1:A:352:TRP:HZ3	1.69	0.57
1:B:138:CYS:SG	3:B:402:COA:S1P	3.02	0.57
1:D:119:ALA:HA	1:D:124:LEU:HG	1.85	0.57
1:D:185:THR:HA	2:D:401:PLM:HA1	1.87	0.57
1:A:35:GLU:OE2	1:A:39:ARG:NH1	2.38	0.56
1:A:325:GLU:C	1:A:327:ARG:H	2.09	0.56
1:A:42:HIS:NE2	1:A:185:THR:HG23	2.20	0.56
1:A:253:LEU:HD11	1:A:337:LEU:HD11	1.87	0.55
1:C:166:GLU:HG3	1:C:312:SER:HB3	1.88	0.55
1:B:310:ASN:ND2	1:B:312:SER:H	2.05	0.54
1:C:78:ASP:OD1	1:C:121:ARG:NH1	2.41	0.54
1:D:147:ARG:NH1	1:D:150:ASP:OD2	2.41	0.54
1:C:159:VAL:HG22	1:C:198:VAL:HG12	1.89	0.53
1:A:28:PHE:HE2	4:A:401:14U:HAA	1.73	0.53
1:A:230:TRP:HH2	4:A:401:14U:HAP	1.73	0.53
1:B:255:ASN:O	1:B:259:THR:HG23	2.09	0.53
1:D:182:LEU:O	1:D:185:THR:HG22	2.08	0.53
1:A:203:ALA:HA	1:A:206:VAL:HG12	1.89	0.53
1:C:319:ILE:O	1:C:323:THR:HG22	2.08	0.52
1:A:206:VAL:HG22	5:A:530:HOH:O	2.09	0.52
1:D:178:THR:HG23	1:D:181:SER:H	1.74	0.52
1:C:84:LEU:HD23	1:C:122:LEU:HD12	1.92	0.51
1:D:301:THR:HB	1:D:319:ILE:HD13	1.93	0.51
1:B:166:GLU:HG3	1:B:312:SER:HB3	1.91	0.51
1:B:269:ASP:N	1:B:269:ASP:OD1	2.44	0.50
1:B:301:THR:HB	1:B:319:ILE:HD13	1.93	0.50
1:A:149:ARG:NH1	1:A:215:ASP:OD1	2.44	0.50
1:B:327:ARG:HG3	1:B:327:ARG:NH2	2.26	0.50
1:D:25:PHE:O	1:D:31:LEU:CD1	2.59	0.50
1:D:27:GLU:OE2	1:D:32:LYS:NZ	2.44	0.50
1:D:3:VAL:HG11	1:D:203:ALA:HB2	1.94	0.50
1:C:230:TRP:CH2	2:C:401:PLM:H52	2.47	0.50
1:C:275:VAL:HG22	1:C:323:THR:HG21	1.94	0.50
1:D:99:ASP:OD1	1:D:125:ARG:NH2	2.45	0.49
1:D:136:LEU:HB2	1:D:140:ALA:HB2	1.94	0.49
1:B:310:ASN:C	1:B:310:ASN:HD22	2.15	0.49
1:A:28:PHE:CE2	4:A:401:14U:HAA	2.47	0.49
1:D:178:THR:CG2	1:D:181:SER:HB2	2.42	0.49
1:D:253:LEU:O	1:D:257:VAL:HG12	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:THR:CG2	1:C:167:LEU:H	2.16	0.49
1:C:4:ILE:HD12	1:C:211:PRO:HG2	1.94	0.49
1:D:28:PHE:HB2	1:D:31:LEU:HD11	1.93	0.49
1:D:74:GLU:OE2	1:D:75:LYS:NZ	2.37	0.49
1:C:136:LEU:O	1:C:139:VAL:HG12	2.12	0.48
1:D:230:TRP:CH2	2:D:401:PLM:H52	2.46	0.48
1:B:310:ASN:HD22	1:B:312:SER:H	1.62	0.48
1:A:166:GLU:CG	1:A:312:SER:HB3	2.41	0.48
1:C:1:MET:HG2	1:C:153:ARG:CG	2.43	0.48
1:A:23:ASP:OD1	1:A:39:ARG:NH2	2.46	0.48
1:A:15:ARG:HD3	1:A:51:HIS:CE1	2.49	0.48
1:C:100:MET:HB2	1:C:129:ARG:HB2	1.94	0.48
1:B:230:TRP:CH2	4:B:401:14U:HAR	2.48	0.48
1:A:280:GLY:O	1:A:284:ILE:HG13	2.14	0.47
1:C:241:LEU:HD13	3:C:402:COA:N6A	2.29	0.47
1:A:35:GLU:O	1:A:39:ARG:HG3	2.13	0.47
1:A:10:ALA:O	1:A:11:LEU:HD23	2.14	0.47
1:A:14:HIS:HB3	1:A:16:TYR:CE1	2.49	0.47
1:D:72:PHE:HA	1:D:170:LEU:HD23	1.95	0.47
1:D:253:LEU:HD11	1:D:337:LEU:HD11	1.97	0.47
1:C:231:ASP:HB3	1:C:238:ARG:NH2	2.30	0.47
1:D:147:ARG:HA	1:D:147:ARG:HD3	1.67	0.46
1:A:211:PRO:HB3	1:A:352:TRP:CE3	2.50	0.46
1:C:261:LEU:HD11	1:C:271:ILE:HD11	1.98	0.46
1:B:218:SER:O	1:A:127:ASP:HA	2.15	0.46
1:C:201:ARG:HH11	1:A:353:ARG:NH2	2.14	0.46
1:B:14:HIS:HB2	1:B:52:LEU:O	2.16	0.46
1:B:310:ASN:HD22	1:B:311:LEU:N	2.14	0.46
1:A:275:VAL:HB	1:A:336:MET:HA	1.97	0.46
1:B:100:MET:HB2	1:B:129:ARG:HB2	1.98	0.46
1:C:230:TRP:HH2	2:C:401:PLM:H52	1.80	0.46
1:A:351:ARG:NH2	1:A:351:ARG:CG	2.72	0.45
1:C:77:VAL:O	1:C:81:VAL:HG13	2.17	0.45
1:A:335:LEU:HA	1:A:335:LEU:HD12	1.70	0.45
1:D:149:ARG:HD2	1:D:213:ILE:HG22	1.97	0.45
1:B:198:VAL:HG13	1:B:202:ARG:HB3	1.98	0.45
1:B:182:LEU:O	1:B:185:THR:HG22	2.17	0.45
1:D:42:HIS:NE2	1:D:185:THR:HG23	2.32	0.45
1:B:265:ARG:HB2	1:B:265:ARG:HH21	1.82	0.44
1:C:103:THR:HG21	1:C:114:LEU:HB2	1.99	0.44
1:B:135:GLY:HA2	1:A:111:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:SER:OG	1:C:313:SER:OG	2.27	0.44
1:B:127:ASP:HA	1:A:218:SER:O	2.18	0.44
1:D:214:LEU:HD22	1:A:205:GLN:HE22	1.81	0.44
1:D:182:LEU:HA	1:D:185:THR:HG22	2.00	0.44
1:A:271:ILE:HD11	1:A:274:TRP:CD2	2.53	0.44
1:B:84:LEU:HD23	1:B:122:LEU:HD12	2.00	0.44
1:C:157:ASP:OD2	1:A:353:ARG:NH2	2.50	0.44
1:C:204:GLU:H	1:C:204:GLU:HG3	1.59	0.44
1:D:41:LEU:HA	1:D:41:LEU:HD12	1.86	0.44
1:A:298:LEU:O	1:A:302:TRP:HD1	2.01	0.44
1:A:328:PRO:HB2	1:A:329:PRO:HD2	2.00	0.44
1:C:15:ARG:NH1	1:C:307:GLU:OE1	2.51	0.44
4:B:401:14U:HAL	4:B:401:14U:HAOA	1.67	0.43
1:D:14:HIS:HB2	1:D:52:LEU:O	2.18	0.43
1:D:274:TRP:CZ3	1:D:335:LEU:HD23	2.53	0.43
1:D:170:LEU:HA	1:D:170:LEU:HD12	1.75	0.43
1:B:108:GLY:HA2	5:B:513:HOH:O	2.18	0.43
1:D:257:VAL:HG22	1:D:261:LEU:HD22	2.00	0.43
1:A:53:VAL:HG13	1:A:54:LEU:HD13	2.00	0.43
1:C:37:ILE:HG12	1:C:41:LEU:HD22	2.01	0.43
1:D:211:PRO:HG3	1:D:352:TRP:CZ3	2.54	0.43
1:A:341:PRO:HD3	4:A:401:14U:HABB	2.01	0.43
1:C:1:MET:HG2	1:C:153:ARG:HG3	1.99	0.43
1:C:81:VAL:HG12	1:C:118:ILE:HG23	2.01	0.43
1:D:336:MET:HB2	1:D:348:VAL:HB	2.01	0.43
1:A:271:ILE:HD11	1:A:274:TRP:CE2	2.53	0.43
1:B:134:PHE:HB3	1:A:134:PHE:HB3	2.00	0.43
1:C:106:VAL:HG22	1:C:230:TRP:HE1	1.84	0.43
1:A:143:ALA:O	1:A:147:ARG:HG2	2.19	0.42
1:D:220:LEU:HB2	5:C:506:HOH:O	2.18	0.42
1:C:201:ARG:NH1	1:A:353:ARG:NH2	2.67	0.42
1:D:62:LEU:HD23	1:D:62:LEU:HA	1.91	0.42
1:B:98:ILE:HD12	1:B:124:LEU:HD22	2.01	0.42
1:B:251:ARG:NH2	1:B:252:TYR:OH	2.52	0.42
1:C:1:MET:CE	1:C:153:ARG:HG2	2.49	0.42
2:C:401:PLM:H92	2:C:401:PLM:H61	1.78	0.42
1:D:12:PRO:O	1:D:51:HIS:ND1	2.44	0.42
1:B:42:HIS:NE2	1:B:185:THR:HG23	2.35	0.42
1:D:172:TYR:HA	1:D:175:VAL:HG13	2.01	0.42
1:D:227:ILE:HG13	1:D:248:LEU:HD12	2.01	0.42
1:A:49:GLY:HA2	5:A:523:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:GLU:C	1:A:327:ARG:N	2.73	0.42
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.88	0.42
1:D:280:GLY:O	1:D:284:ILE:HG13	2.19	0.42
1:D:311:LEU:HB3	1:D:314:ALA:HB3	2.01	0.42
1:A:94:ARG:HG2	1:A:97:ASP:OD2	2.19	0.42
1:C:304:SER:O	1:C:308:ILE:HG12	2.19	0.42
1:C:32:LYS:NZ	1:C:35:GLU:OE2	2.37	0.42
1:A:12:PRO:O	1:A:51:HIS:HD2	2.03	0.41
1:B:125:ARG:NH2	1:B:127:ASP:OD1	2.53	0.41
1:C:253:LEU:HD21	1:C:337:LEU:HD21	2.02	0.41
1:D:230:TRP:HA	1:D:230:TRP:CE3	2.56	0.41
1:C:14:HIS:HB2	1:C:52:LEU:O	2.21	0.41
1:A:326:LYS:O	1:A:327:ARG:C	2.59	0.41
1:B:103:THR:HG22	1:B:132:PRO:HA	2.01	0.41
1:C:112:PRO:HD2	1:C:117:ARG:NH1	2.35	0.41
1:C:283:VAL:O	1:C:287:VAL:HG13	2.21	0.41
1:D:85:LEU:HD23	1:D:85:LEU:HA	1.96	0.41
1:C:35:GLU:O	1:C:39:ARG:HG3	2.20	0.41
1:C:185:THR:HA	2:C:401:PLM:HB2	2.02	0.41
1:B:72:PHE:CD2	1:B:108:GLY:HA3	2.55	0.41
1:C:261:LEU:HD13	1:C:261:LEU:HA	1.85	0.41
1:D:11:LEU:HD21	1:D:318:HIS:CE1	2.56	0.41
1:D:93:LEU:HD21	1:D:206:VAL:HG21	2.03	0.40
1:B:261:LEU:HA	1:B:261:LEU:HD12	1.89	0.40
1:D:111:VAL:HG22	1:C:135:GLY:HA2	2.02	0.40
1:D:57:GLN:O	1:D:60:PRO:HD2	2.21	0.40
1:C:110:ALA:O	1:C:113:SER:HA	2.22	0.40
1:A:136:LEU:HB2	1:A:140:ALA:HB2	2.03	0.40
1:B:328:PRO:HG2	1:B:352:TRP:CD2	2.56	0.40
1:C:3:VAL:HB	1:C:212:ASP:OD1	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	351/353 (99%)	333 (95%)	14 (4%)	4 (1%)	14	4
1	B	350/353 (99%)	335 (96%)	13 (4%)	2 (1%)	25	12
1	C	351/353 (99%)	338 (96%)	12 (3%)	1 (0%)	41	27
1	D	350/353 (99%)	335 (96%)	14 (4%)	1 (0%)	41	27
All	All	1402/1412 (99%)	1341 (96%)	53 (4%)	8 (1%)	25	12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	278	PRO
1	C	2	SER
1	A	327	ARG
1	A	352	TRP
1	B	327	ARG
1	A	14	HIS
1	D	210	GLY
1	A	206	VAL

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	281/281 (100%)	242 (86%)	39 (14%)	3	0
1	B	280/281 (100%)	245 (88%)	35 (12%)	4	0
1	C	281/281 (100%)	248 (88%)	33 (12%)	5	0
1	D	280/281 (100%)	227 (81%)	53 (19%)	1	0
All	All	1122/1124 (100%)	962 (86%)	160 (14%)	3	0

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3	VAL
1	D	19	SER
1	D	20	GLU
1	D	31	LEU
1	D	32	LYS
1	D	33	GLU
1	D	36	GLU
1	D	41	LEU
1	D	54	LEU
1	D	57	GLN
1	D	62	LEU
1	D	74	GLU
1	D	79	LEU
1	D	84	LEU
1	D	88	LEU
1	D	89	ASP
1	D	90	ASP
1	D	109	VAL
1	D	115	ASP
1	D	139	VAL
1	D	147	ARG
1	D	148	LEU
1	D	161	VAL
1	D	164	SER
1	D	170	LEU
1	D	176	LYS
1	D	180	SER
1	D	181	SER
1	D	187	LEU
1	D	220	LEU
1	D	230	TRP
1	D	231	ASP
1	D	237	LEU
1	D	245	LEU
1	D	251	ARG
1	D	261	LEU
1	D	269	ASP
1	D	298	LEU
1	D	299	GLU
1	D	300	LEU
1	D	301	THR
1	D	303	ARG
1	D	305	LEU

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Mol	Chain	Res	Type
1	D	307	GLU
1	D	308	ILE
1	D	311	LEU
1	D	321	ARG
1	D	325	GLU
1	D	327	ARG
1	D	345	THR
1	D	347	LEU
1	D	350	LEU
1	D	353	ARG
1	C	1	MET
1	C	2	SER
1	C	3	VAL
1	C	17	SER
1	C	41	LEU
1	C	79	LEU
1	C	100	MET
1	C	103	THR
1	C	107	THR
1	C	114	LEU
1	C	115	ASP
1	C	147	ARG
1	C	148	LEU
1	C	153	ARG
1	C	180	SER
1	C	204	GLU
1	C	223	ASP
1	C	241	LEU
1	C	255	ASN
1	C	265	ARG
1	C	266	LEU
1	C	268	LYS
1	C	270	ASP
1	C	287	VAL
1	C	300	LEU
1	C	301	THR
1	C	307	GLU
1	C	311	LEU
1	C	326	LYS
1	C	327	ARG
1	C	345	THR
1	C	351	ARG

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Mol	Chain	Res	Type
1	C	353	ARG
1	B	15	ARG
1	B	37	ILE
1	B	46	LYS
1	B	79	LEU
1	B	85	LEU
1	B	88	LEU
1	B	94	ARG
1	B	100	MET
1	B	103	THR
1	B	114	LEU
1	B	115	ASP
1	B	139	VAL
1	B	147	ARG
1	B	148	LEU
1	B	153	ARG
1	B	170	LEU
1	B	178	THR
1	B	180	SER
1	B	185	THR
1	B	217	ARG
1	B	224	SER
1	B	237	LEU
1	B	249	ILE
1	B	251	ARG
1	B	261	LEU
1	B	265	ARG
1	B	269	ASP
1	B	282	LYS
1	B	300	LEU
1	B	301	THR
1	B	305	LEU
1	B	310	ASN
1	B	315	SER
1	B	347	LEU
1	B	353	ARG
1	A	1	MET
1	A	2	SER
1	A	74	GLU
1	A	84	LEU
1	A	88	LEU
1	A	94	ARG

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Mol	Chain	Res	Type
1	A	103	THR
1	A	114	LEU
1	A	115	ASP
1	A	148	LEU
1	A	178	THR
1	A	181	SER
1	A	185	THR
1	A	187	LEU
1	A	204	GLU
1	A	206	VAL
1	A	207	ARG
1	A	230	TRP
1	A	237	LEU
1	A	240	ARG
1	A	248	LEU
1	A	251	ARG
1	A	255	ASN
1	A	262	ASP
1	A	267	THR
1	A	268	LYS
1	A	269	ASP
1	A	271	ILE
1	A	293	LEU
1	A	296	GLU
1	A	298	LEU
1	A	300	LEU
1	A	325	GLU
1	A	326	LYS
1	A	327	ARG
1	A	328	PRO
1	A	330	SER
1	A	350	LEU
1	A	351	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	310	ASN
1	A	51	HIS

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](#)

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
4	14U	A	401	1	19,20,21	0.70	1 (5%)	18,21,23	1.70	3 (16%)
4	14U	B	401	1	19,20,21	0.88	1 (5%)	18,21,23	2.08	4 (22%)
2	PLM	D	401	-	14,17,17	0.46	0	13,17,17	0.78	0
2	PLM	C	401	-	14,17,17	0.53	0	13,17,17	1.11	0
3	COA	B	402	-	41,50,50	2.06	9 (21%)	52,75,75	1.54	7 (13%)
3	COA	C	402	-	41,50,50	2.03	9 (21%)	52,75,75	1.34	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	14U	A	401	1	-	0/19/21/23	-
4	14U	B	401	1	-	0/19/21/23	-
2	PLM	D	401	-	-	0/13/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLM	C	401	-	-	0/13/15/15	-
3	COA	B	402	-	-	10/44/64/64	0/3/3/3
3	COA	C	402	-	-	11/44/64/64	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	COA	C9P-N8P	6.65	1.48	1.33
3	B	402	COA	C9P-N8P	6.58	1.48	1.33
3	B	402	COA	C5P-N4P	6.09	1.47	1.33
3	C	402	COA	C5P-N4P	5.66	1.46	1.33
3	C	402	COA	P2A-O4A	4.98	1.68	1.50
3	B	402	COA	P2A-O4A	4.94	1.68	1.50
3	C	402	COA	C6A-N6A	3.42	1.46	1.34
3	B	402	COA	C6A-N6A	3.35	1.46	1.34
3	C	402	COA	P2A-O5A	3.00	1.69	1.55
3	B	402	COA	C2B-C1B	-2.75	1.49	1.53
3	C	402	COA	C2A-N3A	2.74	1.36	1.32
3	B	402	COA	P2A-O6A	2.61	1.69	1.59
3	B	402	COA	P2A-O5A	2.59	1.67	1.55
3	B	402	COA	C2A-N3A	2.55	1.36	1.32
3	C	402	COA	C2B-C1B	-2.38	1.50	1.53
3	B	402	COA	O2B-C2B	-2.34	1.37	1.43
3	C	402	COA	O2B-C2B	-2.25	1.37	1.43
3	C	402	COA	P2A-O6A	2.24	1.68	1.59
4	A	401	14U	CAB-CAU	-2.18	1.51	1.54
4	B	401	14U	CAS-CAT	2.15	1.54	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	COA	N3A-C2A-N1A	-6.18	119.02	128.68
3	C	402	COA	N3A-C2A-N1A	-5.76	119.67	128.68
4	B	401	14U	CAB-CAU-CAE	-5.27	105.41	110.83
4	A	401	14U	CAB-CAU-CAT	-4.50	102.35	109.19
4	B	401	14U	CAB-CAU-CAT	-4.05	103.03	109.19
3	B	402	COA	C6P-C5P-N4P	3.78	122.79	116.42
4	B	401	14U	CAR-CAS-CAT	-3.56	108.42	114.60
4	A	401	14U	CAB-CAU-CAE	-3.43	107.29	110.83
3	B	402	COA	C7P-C6P-C5P	-3.28	106.90	112.36
3	B	402	COA	O5P-C5P-C6P	-2.66	117.14	122.02
4	A	401	14U	CAR-CAS-CAT	-2.49	110.27	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
3	B	402	COA	O5A-P2A-O6A	2.47	119.22	107.75
3	B	402	COA	C2A-N1A-C6A	2.35	122.77	118.75
3	B	402	COA	CEP-CBP-CAP	2.29	112.80	108.82
3	C	402	COA	O6A-P2A-O4A	2.25	117.86	109.07
4	B	401	14U	OAD-CAT-CAU	-2.13	118.02	120.93

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	COA	C5B-O5B-P1A-O1A
3	B	402	COA	CCP-O6A-P2A-O3A
3	B	402	COA	CCP-O6A-P2A-O4A
3	B	402	COA	CAP-CBP-CCP-O6A
3	B	402	COA	S1P-C2P-C3P-N4P
3	C	402	COA	CCP-O6A-P2A-O5A
3	C	402	COA	CDP-CBP-CCP-O6A
3	C	402	COA	CEP-CBP-CCP-O6A
3	C	402	COA	CAP-CBP-CCP-O6A
3	C	402	COA	S1P-C2P-C3P-N4P
3	C	402	COA	C3B-C4B-C5B-O5B
3	B	402	COA	CDP-CBP-CCP-O6A
3	B	402	COA	CEP-CBP-CCP-O6A
3	C	402	COA	O4B-C4B-C5B-O5B
3	B	402	COA	C5P-C6P-C7P-N8P
3	B	402	COA	C5B-O5B-P1A-O3A
3	C	402	COA	CCP-O6A-P2A-O3A
3	B	402	COA	C5B-O5B-P1A-O2A
3	C	402	COA	CCP-O6A-P2A-O4A
3	C	402	COA	C5P-C6P-C7P-N8P
3	C	402	COA	C5B-O5B-P1A-O1A

There are no ring outliers.

6 monomers are involved in 21 short contacts:

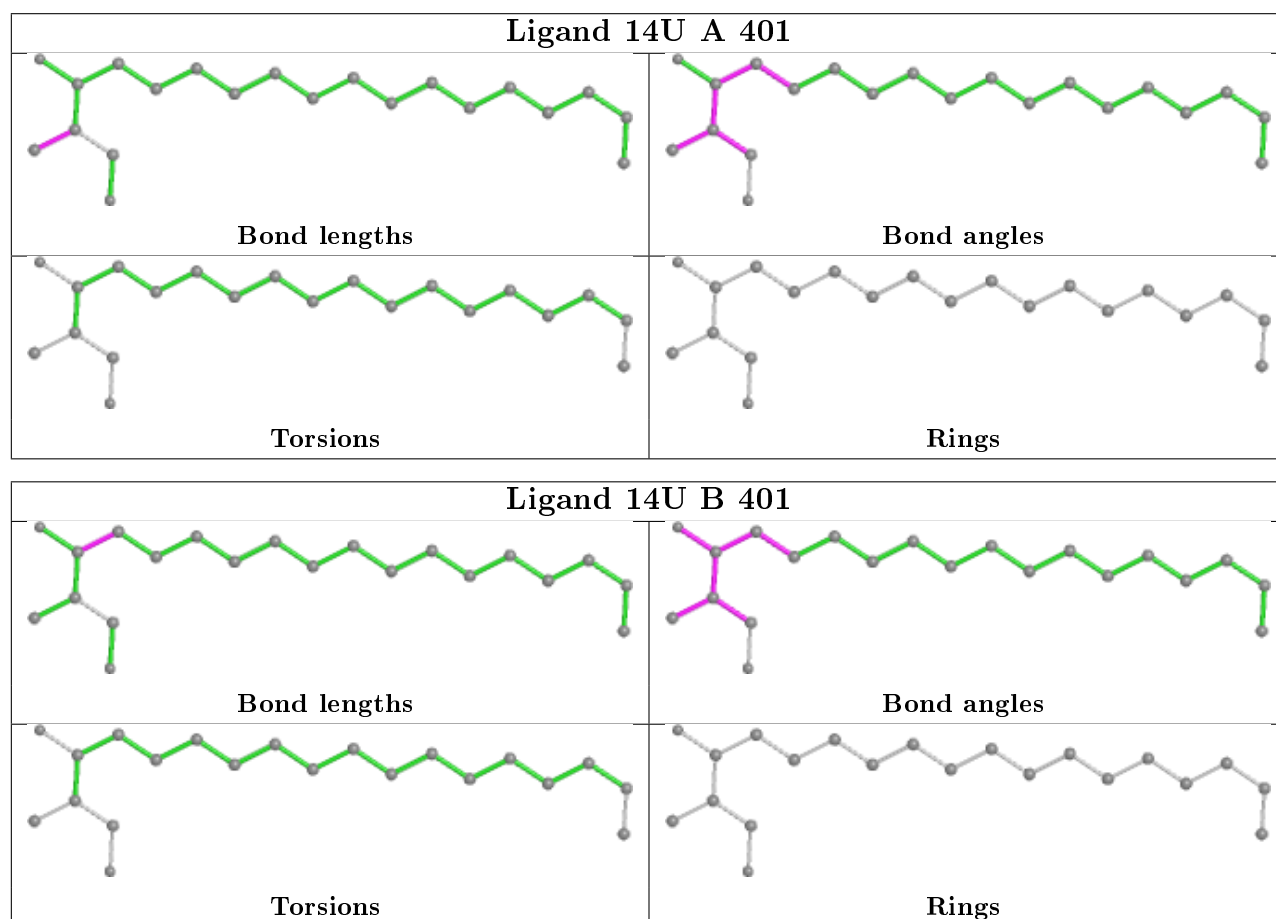
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	14U	6	0
4	B	401	14U	3	0
2	D	401	PLM	5	0
2	C	401	PLM	5	0
3	B	402	COA	1	0

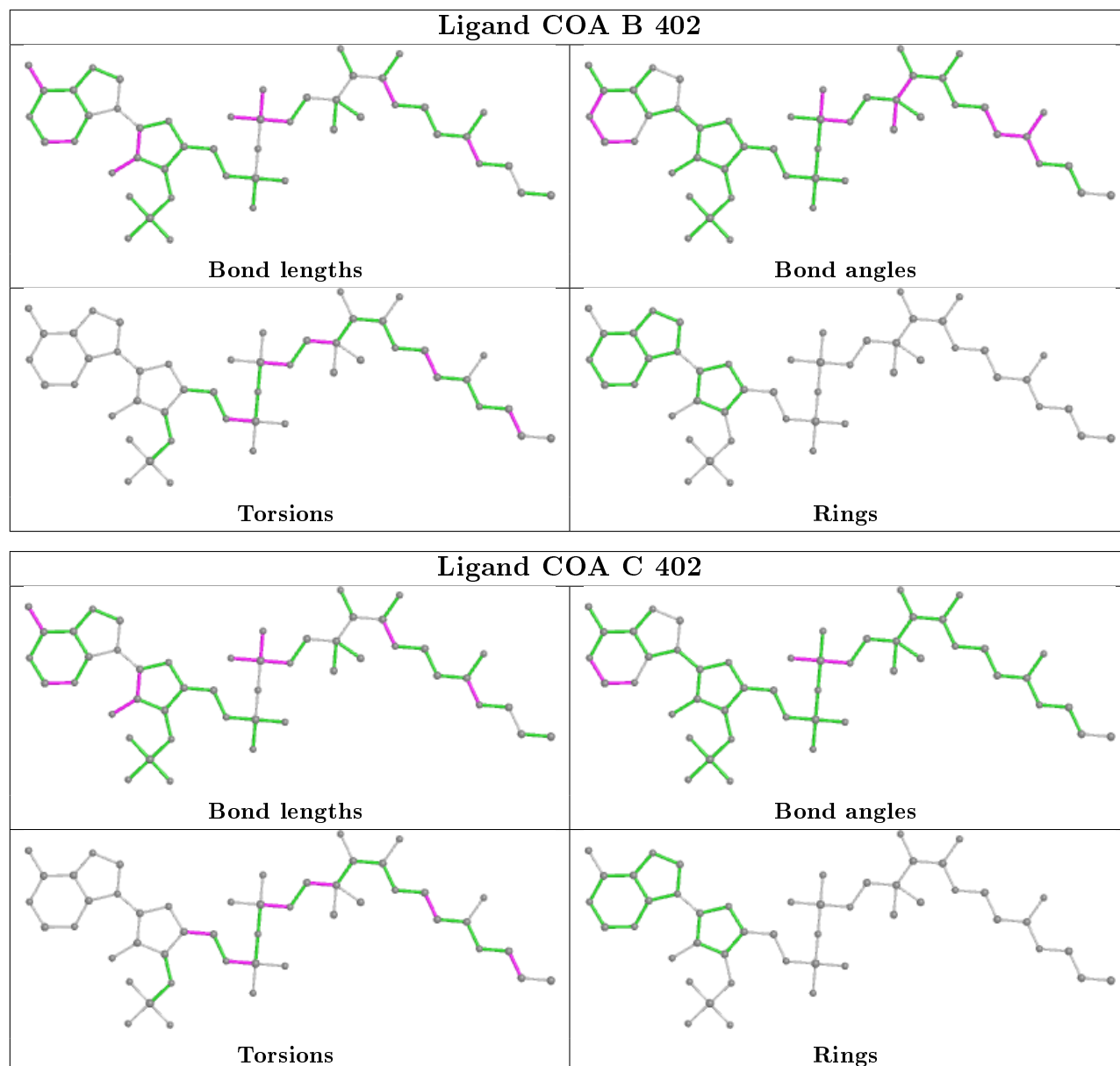
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	COA	1	0

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 than 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.





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(Å ²)	Q<0.9
1	A	353/353 (100%)	0.40	17 (4%) 30 28	35, 51, 69, 80	0
1	B	352/353 (99%)	0.22	7 (1%) 65 64	31, 47, 66, 76	0
1	C	353/353 (100%)	0.26	17 (4%) 30 28	38, 55, 71, 79	0
1	D	352/353 (99%)	0.28	17 (4%) 30 28	38, 56, 71, 81	0
All	All	1410/1412 (99%)	0.29	58 (4%) 37 34	31, 53, 71, 81	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	31	LEU	6.2
1	C	267	THR	4.1
1	D	25	PHE	4.0
1	C	1	MET	3.7
1	A	271	ILE	3.6
1	A	292	ALA	3.6
1	D	30	GLY	3.6
1	D	37	ILE	3.5
1	B	265	ARG	3.4
1	A	1	MET	3.4
1	A	274	TRP	3.4
1	C	271	ILE	3.2
1	D	353	ARG	3.1
1	B	295	PRO	2.9
1	A	264	HIS	2.9
1	A	124	LEU	2.8
1	C	278	PRO	2.8
1	C	260	PHE	2.8
1	C	206	VAL	2.8
1	C	266	LEU	2.8
1	B	353	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	11	LEU	2.7
1	B	207	ARG	2.6
1	C	265	ARG	2.6
1	C	330	SER	2.6
1	A	30	GLY	2.6
1	B	209	GLY	2.5
1	D	14	HIS	2.5
1	A	353	ARG	2.5
1	C	207	ARG	2.5
1	C	335	LEU	2.5
1	C	293	LEU	2.4
1	C	205	GLN	2.4
1	B	329	PRO	2.4
1	D	205	GLN	2.4
1	D	26	VAL	2.4
1	A	298	LEU	2.3
1	D	29	PRO	2.3
1	C	275	VAL	2.3
1	D	32	LYS	2.3
1	A	352	TRP	2.3
1	D	207	ARG	2.3
1	B	352	TRP	2.2
1	A	269	ASP	2.2
1	D	45	ALA	2.2
1	A	116	ALA	2.2
1	D	38	ILE	2.2
1	A	265	ARG	2.2
1	D	40	ARG	2.2
1	A	112	PRO	2.2
1	D	352	TRP	2.2
1	C	261	LEU	2.1
1	C	272	GLY	2.1
1	A	249	ILE	2.1
1	D	172	TYR	2.1
1	A	77	VAL	2.0
1	A	327	ARG	2.0
1	C	269	ASP	2.0

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 [i](#)

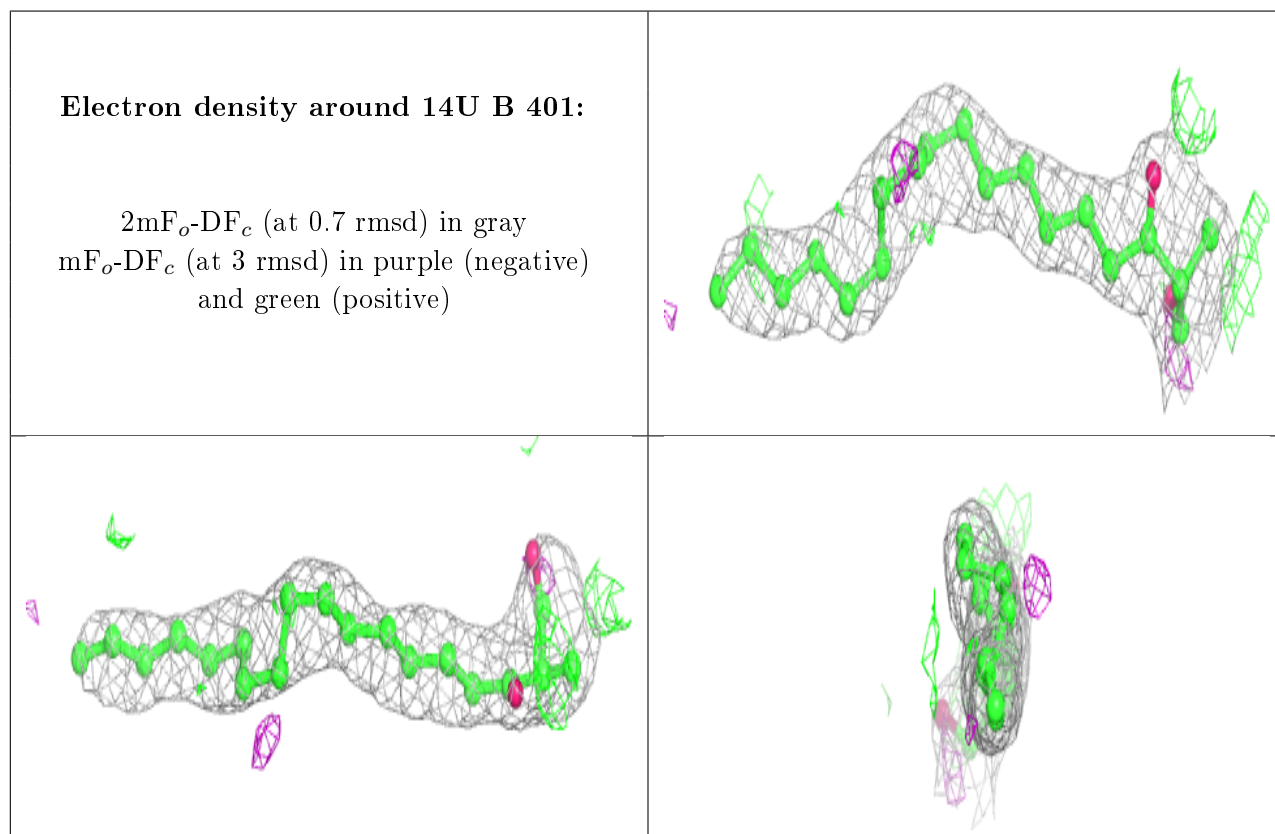
There are no carbohydrates in this entry.

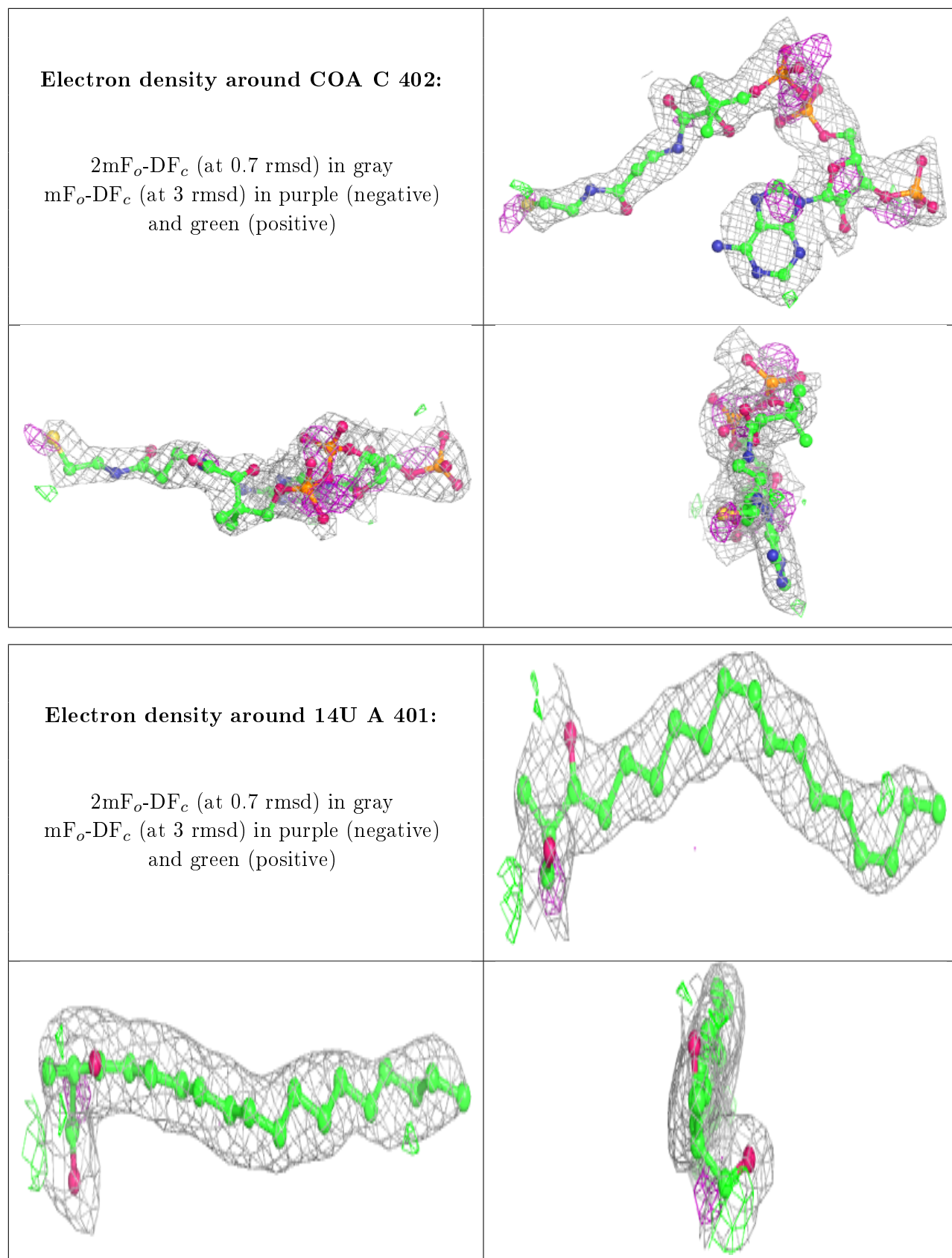
6.4 Ligands [i](#)

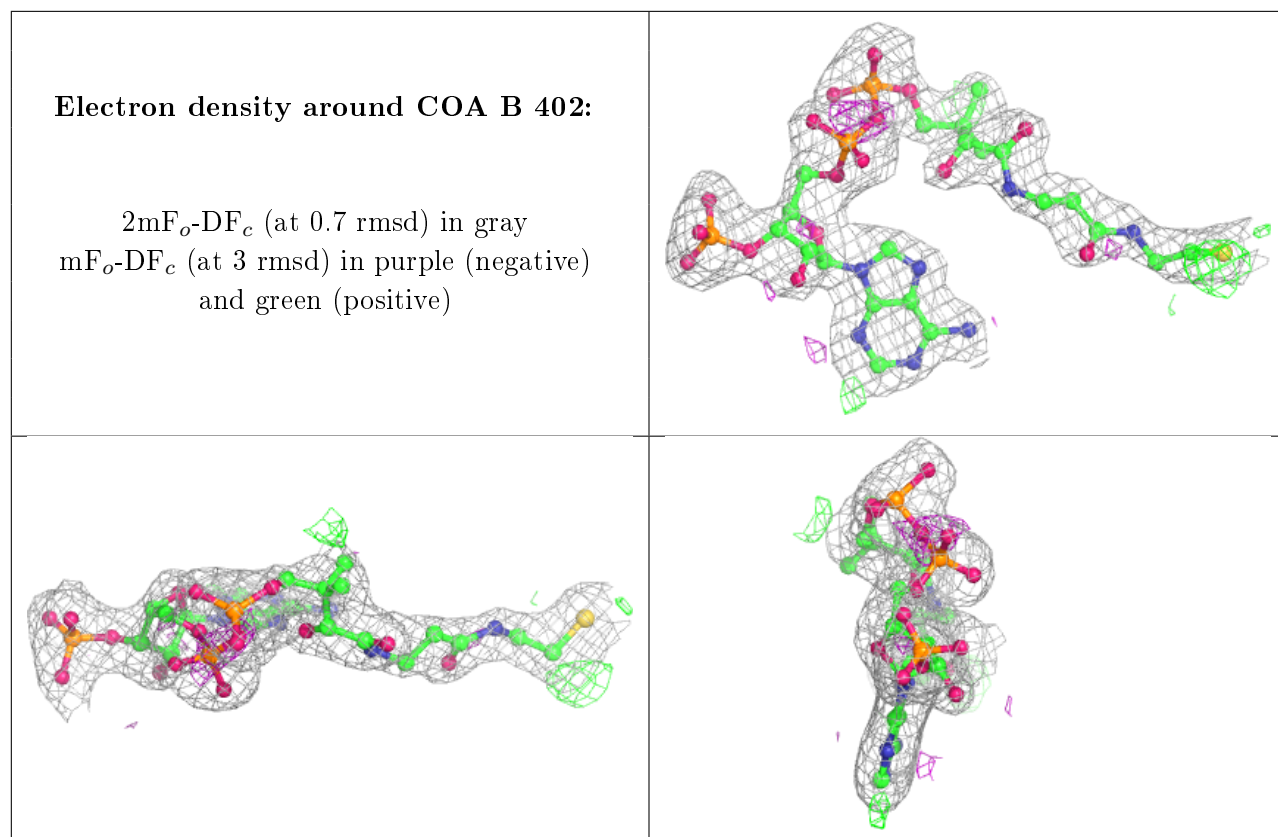
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLM	D	401	18/18	0.79	0.22	53,59,66,68	0
2	PLM	C	401	18/18	0.79	0.20	51,55,66,67	0
4	14U	B	401	21/22	0.82	0.17	37,44,56,62	0
3	COA	C	402	48/48	0.83	0.23	61,76,88,94	0
4	14U	A	401	21/22	0.87	0.15	38,47,53,54	0
3	COA	B	402	48/48	0.92	0.11	47,62,71,75	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.







6.5 Other polymers [i](#)

There are no such residues in this entry.