WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2024 – 05:00 AM EST

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)

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	Percentile Ranks	Value
Rfree		0.284
Clashscore		9
Ramachandran outliers		0.6%
Sidechain outliers		14.3%
RSRZ outliers		1.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▐ Percentile relative to X-ray structures of similar resolution
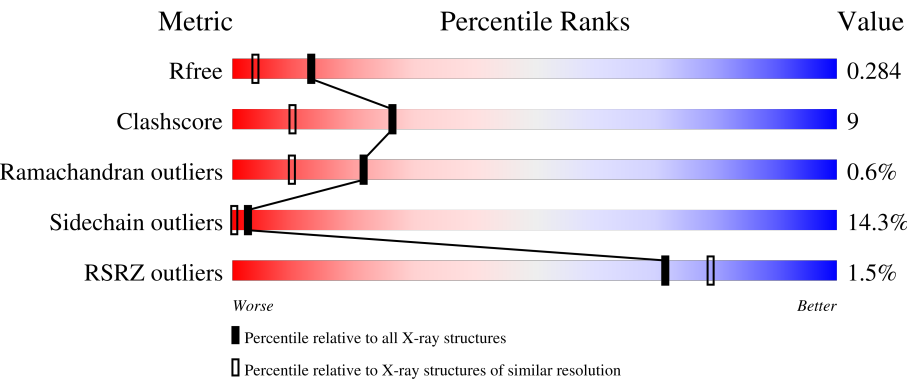
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol	Chain	Length	Quality of chain
1	A	353	2% · 73% · 22% · ·
1	B	353	% · 79% · 18% ·
1	C	353	% · 75% · 22% ·
1	D	353	2% · 68% · 26% · 6%

2 Entry composition ⓘ

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
1	D	352	Total	C	N	O	S	0	0	0
			2642	1671	469	494	8			
1	C	353	Total	C	N	O	S	0	0	0
			2649	1676	470	494	9			
1	B	352	Total	C	N	O	S	0	0	0
			2641	1671	469	493	8			
1	A	353	Total	C	N	O	S	0	0	0
			2650	1676	470	495	9			

- Molecule 2 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).
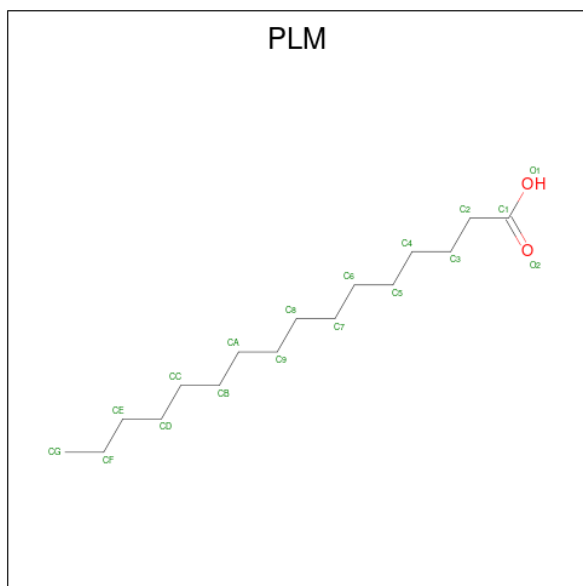
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			18	16	2		
2	C	1	Total	C	O	0	0
			18	16	2		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).
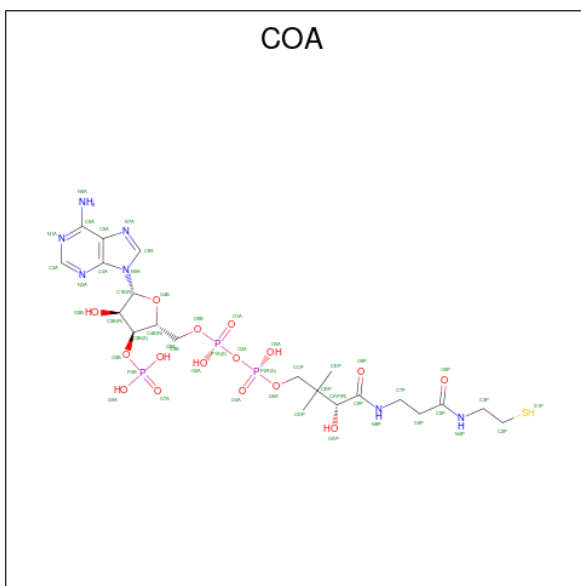
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is (2S)-2-methyl-3-oxooctadecanoic acid (three-letter code: 14U) (formula: $C_{19}H_{36}O_3$).
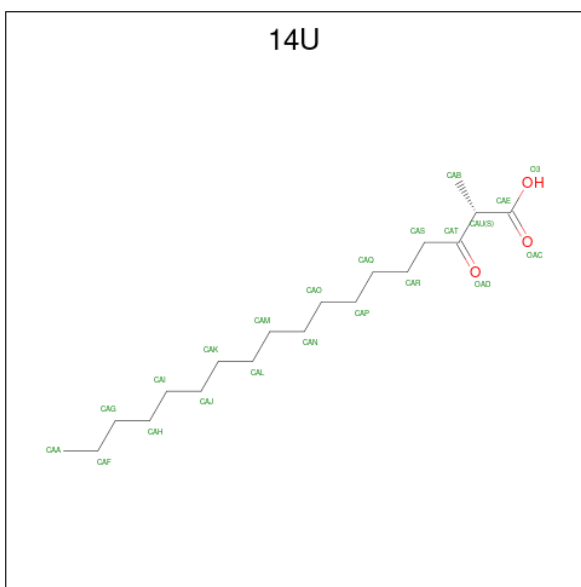
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 21	C 19	O 2	0	0
4	A	1	Total 21	C 19	O 2	0	0

- Molecule 5 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

Chain D:

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

Chain C:

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

Chain B:

R147 L148 R153 E166 S169 L170 T178 V179 S180 S181 L182 T185 V198 R202 R217 S218 S224 W230 L237 I249 E250 R251 Y252 N255 T259 F260 L261 R265 D269 P278 G279 K282 P295 E296 L300 T301 L305 N310

L311 S312 S315 I319 R327 P328 F343 L347 W352 R353

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

Chain A:

M1 S2 A10 L11 P12 P13 H14 R15 Y16 S17 Q18 D23 F28 E35 R39 H42 G49 R50 H51 L52 V53 L54 E74 L84 L88 R94 D97 T103 V111 L114 D115 A119 L124 D127 F134 G135 L136 A140 A143

R147 L148 R149 E166 S169 T178 S181 L182 T185 A186 L187 A203 E204 Q205 V206 R207 A208 G209 G210 P211 D215 S218 S219 W230 L237 R240 L248 R251 Y252 L253 A254 N255 D262 A263 H264 T267 K268 D269 D270 I271 W274 V275

G279 G280 I284 L293 E296 A297 L298 E299 L300 T301 W302 L311 S312 S313 A314 I324 E325 K326 R327 P328 P329 S330 L335 M336 L337 P341 T345 L350 R351 W352 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 48.63Å 193.66Å 90.00° 97.57° 90.00°	Depositor
Resolution (Å)	44.80 – 1.83	Depositor
	44.80 – 1.83	EDS
% Data completeness	77.4 (44.80-1.83)	Depositor
(in resolution range)	77.4 (44.80-1.83)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 1.83Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.234 , 0.289	Depositor
	0.229 , 0.284	DCC
R_{free} test set	4557 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 26.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10941	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage'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.*

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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: PLM, COA, 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:D:169:SER:HA	2:D:401:PLM:HB1	1.79	0.65
1:C:169:SER:HA	2:C:401:PLM:HA2	1.77	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:HH21	1:B:327:ARG:HG3	1.62	0.64
1:D:230:TRP:HH2	2:D:401:PLM:H52	1.62	0.63
1:A:311:LEU:HB3	1:A:314:ALA:HB3	1.79	0.63
1:C:119:ALA:HA	1:C:124:LEU:HG	1.80	0.63
1:C:301:THR:HB	1:C:319:ILE:HD13	1.81	0.62
1:B:178:THR:HG22	1:B:181:SER:H	1.64	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:B:119:ALA:HA	1:B:124:LEU:HG	1.82	0.60
1:A:351:ARG:HH21	1:A:351:ARG:CG	2.07	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:HG2	1:A:351:ARG:NH2	2.03	0.58
1:B:138:CYS:SG	3:B:402:COA:S1P	3.02	0.57
1:A:324:ILE:HG12	1:A:352:TRP:HZ3	1.69	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:D:182:LEU:O	1:D:185:THR:HG22	2.08	0.53
1:B:255:ASN:O	1:B:259:THR:HG23	2.09	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:D:301:THR:HB	1:D:319:ILE:HD13	1.93	0.51
1:C:84:LEU:HD23	1:C:122:LEU:HD12	1.92	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:D:3:VAL:HG11	1:D:203:ALA:HB2	1.94	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:B:327:ARG:HG3	1:B:327:ARG:NH2	2.26	0.50
1:A:149:ARG:NH1	1:A:215:ASP:OD1	2.44	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:HD22	1:B:310:ASN:C	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:4:ILE:HD12	1:C:211:PRO:HG2	1.94	0.49
1:C:107:THR:CG2	1:C:167:LEU:H	2.16	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:C:1:MET:HG2	1:C:153:ARG:CG	2.43	0.48
1:A:166:GLU:CG	1:A:312:SER:HB3	2.41	0.48
1:C:100:MET:HB2	1:C:129:ARG:HB2	1.94	0.48
1:A:15:ARG:HD3	1:A:51:HIS:CE1	2.49	0.48
1:A:23:ASP:OD1	1:A:39:ARG:NH2	2.46	0.48
1:B:230:TRP:CH2	4:B:401:14U:HAR	2.48	0.48
1:C:241:LEU:HD13	3:C:402:COA:N6A	2.29	0.47
1:A:280:GLY:O	1:A:284:ILE:HG13	2.14	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:HD3	1:D:147:ARG:HA	1.67	0.46
1:C:261:LEU:HD11	1:C:271:ILE:HD11	1.98	0.46
1:A:211:PRO:HB3	1:A:352:TRP:CE3	2.50	0.46
1:C:201:ARG:HH11	1:A:353:ARG:NH2	2.14	0.46
1:B:218:SER:O	1:A:127:ASP:HA	2.15	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:C:230:TRP:HH2	2:C:401:PLM:H52	1.80	0.46
1:B:100:MET:HB2	1:B:129:ARG:HB2	1.98	0.46
1:A:351:ARG:CG	1:A:351:ARG:NH2	2.72	0.45
1:C:77:VAL:O	1:C:81:VAL:HG13	2.17	0.45
1:A:335:LEU:HD12	1:A:335:LEU:HA	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:D:42:HIS:NE2	1:D:185:THR:HG23	2.32	0.45
1:B:182:LEU:O	1:B:185:THR:HG22	2.17	0.45
1:B:265:ARG:HH21	1:B:265:ARG:HB2	1.82	0.44
1:C:103:THR:HG21	1:C:114:LEU:HB2	1.99	0.44
1:C:164:SER:OG	1:C:313:SER:OG	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:GLY:HA2	1:A:111:VAL:HG22	1.98	0.44
1:B:127:ASP:HA	1:A:218:SER:O	2.18	0.44
1:D:182:LEU:HA	1:D:185:THR:HG22	2.00	0.44
1:D:214:LEU:HD22	1:A:205:GLN:HE22	1.81	0.44
1:D:41:LEU:HD12	1:D:41:LEU:HA	1.86	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:B:84:LEU:HD23	1:B:122:LEU:HD12	2.00	0.44
1:A:271:ILE:HD11	1:A:274:TRP:CD2	2.53	0.44
1:C:15:ARG:NH1	1:C:307:GLU:OE1	2.51	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:D:14:HIS:HB2	1:D:52:LEU:O	2.18	0.43
4:B:401:14U:HAL	4:B:401:14U:HAOA	1.67	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:D:257:VAL:HG22	1:D:261:LEU:HD22	2.00	0.43
1:B:108:GLY:HA2	5:B:513:HOH:O	2.18	0.43
1:D:211:PRO:HG3	1:D:352:TRP:CZ3	2.54	0.43
1:C:37:ILE:HG12	1:C:41:LEU:HD22	2.01	0.43
1:A:53:VAL:HG13	1:A:54:LEU:HD13	2.00	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:A:341:PRO:HD3	4:A:401:14U:HABB	2.01	0.43
1:D:336:MET:HB2	1:D:348:VAL:HB	2.01	0.43
1:C:106:VAL:HG22	1:C:230:TRP:HE1	1.84	0.43
1:B:134:PHE:HB3	1:A:134:PHE:HB3	2.00	0.43
1:A:271:ILE:HD11	1:A:274:TRP:CE2	2.53	0.43
1:D:220:LEU:HB2	5:C:506:HOH:O	2.18	0.42
1:A:143:ALA:O	1:A:147:ARG:HG2	2.19	0.42
1:D:62:LEU:HD23	1:D:62:LEU:HA	1.91	0.42
1:C:201:ARG:NH1	1:A:353:ARG:NH2	2.67	0.42
1:C:1:MET:CE	1:C:153:ARG:HG2	2.49	0.42
2:C:401:PLM:H61	2:C:401:PLM:H92	1.78	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:D:12:PRO:O	1:D:51:HIS:ND1	2.44	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:B:42:HIS:NE2	1:B:185:THR:HG23	2.35	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: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:C:182:LEU:HD23	1:C:182:LEU:HA	1.88	0.42
1:A:94:ARG:HG2	1:A:97:ASP:OD2	2.19	0.42
1:C:32:LYS:NZ	1:C:35:GLU:OE2	2.37	0.42
1:C:304:SER:O	1:C:308:ILE:HG12	2.19	0.42
1:B:125:ARG:NH2	1:B:127:ASP:OD1	2.53	0.41
1:A:12:PRO:O	1:A:51:HIS:HD2	2.03	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:D:85:LEU:HD23	1:D:85:LEU:HA	1.96	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:B:103:THR:HG22	1:B:132:PRO:HA	2.01	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:D:11:LEU:HD21	1:D:318:HIS:CE1	2.56	0.41
1:C:261:LEU:HD13	1:C:261:LEU:HA	1.85	0.41
1:B:72:PHE:CD2	1:B:108:GLY:HA3	2.55	0.41
1:D:93:LEU:HD21	1:D:206:VAL:HG21	2.03	0.40
1:D:57:GLN:O	1:D:60:PRO:HD2	2.21	0.40
1:D:111:VAL:HG22	1:C:135:GLY:HA2	2.02	0.40
1:B:261:LEU:HD12	1:B:261:LEU:HA	1.89	0.40
1:C:110:ALA:O	1:C:113:SER:HA	2.22	0.40
1:B:328:PRO:HG2	1:B:352:TRP:CD2	2.56	0.40
1:A:136:LEU:HB2	1:A:140:ALA:HB2	2.03	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	351/353 (99%)	333 (95%)	14 (4%)	4 (1%)	12	4
1	B	350/353 (99%)	335 (96%)	13 (4%)	2 (1%)	22	10
1	C	351/353 (99%)	338 (96%)	12 (3%)	1 (0%)	37	25
1	D	350/353 (99%)	335 (96%)	14 (4%)	1 (0%)	37	25
All	All	1402/1412 (99%)	1341 (96%)	53 (4%)	8 (1%)	22	10

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 ⓘ

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%)	3	0
1	C	281/281 (100%)	248 (88%)	33 (12%)	4	0
1	D	280/281 (100%)	227 (81%)	53 (19%)	1	0
All	All	1122/1124 (100%)	962 (86%)	160 (14%)	2	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

Sometimes 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 ⓘ

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 oligosaccharides 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	B	402	-	43,50,50	2.00	9 (20%)	56,75,75	1.84	9 (16%)
2	PLM	C	401	-	17,17,17	0.92	1 (5%)	17,17,17	1.19	1 (5%)
2	PLM	D	401	-	17,17,17	0.84	0	17,17,17	0.80	0
4	14U	B	401	1	19,20,21	0.93	2 (10%)	20,21,23	2.20	5 (25%)
3	COA	C	402	-	43,50,50	1.97	9 (20%)	56,75,75	1.81	8 (14%)
4	14U	A	401	1	19,20,21	0.74	1 (5%)	20,21,23	1.82	5 (25%)

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	B	402	-	-	10/44/64/64	0/3/3/3
2	PLM	C	401	-	-	0/15/15/15	-
2	PLM	D	401	-	-	2/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	14U	B	401	1	-	2/21/21/23	-
3	COA	C	402	-	-	11/44/64/64	0/3/3/3
4	14U	A	401	1	-	2/21/21/23	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	COA	C9P-N8P	6.19	1.48	1.33
3	B	402	COA	C9P-N8P	6.13	1.48	1.33
3	B	402	COA	C5P-N4P	5.84	1.47	1.33
3	C	402	COA	C5P-N4P	5.42	1.46	1.33
3	C	402	COA	P2A-O4A	5.13	1.68	1.50
3	B	402	COA	P2A-O4A	5.08	1.68	1.50
3	C	402	COA	C6A-N6A	3.48	1.46	1.34
3	B	402	COA	C6A-N6A	3.40	1.46	1.34
3	C	402	COA	P2A-O5A	3.04	1.69	1.55
3	C	402	COA	C2A-N3A	2.85	1.36	1.32
3	B	402	COA	P2A-O6A	2.68	1.69	1.59
3	B	402	COA	C2A-N3A	2.66	1.36	1.32
3	B	402	COA	P2A-O5A	2.62	1.67	1.55
3	C	402	COA	P2A-O3A	2.53	1.62	1.59
2	C	401	PLM	C2-C1	2.48	1.56	1.50
3	B	402	COA	P2A-O3A	2.44	1.62	1.59
4	A	401	14U	CAB-CAU	-2.37	1.51	1.54
3	C	402	COA	P2A-O6A	2.29	1.68	1.59
3	B	402	COA	O2B-C2B	-2.22	1.37	1.43
4	B	401	14U	CAS-CAT	2.19	1.54	1.51
3	C	402	COA	O2B-C2B	-2.13	1.37	1.43
4	B	401	14U	CAB-CAU	-2.01	1.51	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	COA	N3A-C2A-N1A	-7.11	119.02	128.67
3	C	402	COA	N3A-C2A-N1A	-6.63	119.67	128.67
3	B	402	COA	O3A-P2A-O4A	-5.89	92.98	110.70
4	B	401	14U	CAB-CAU-CAE	-5.21	105.41	110.80
3	C	402	COA	O5A-P2A-O3A	-5.19	93.25	107.27
4	A	401	14U	CAB-CAU-CAT	-4.82	102.35	109.31
4	B	401	14U	CAB-CAU-CAT	-4.35	103.03	109.31
3	C	402	COA	O3A-P2A-O4A	-4.34	97.65	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	COA	O4B-C1B-N9A	4.31	114.47	108.75
3	B	402	COA	C4B-O4B-C1B	-3.94	106.32	109.92
4	B	401	14U	CAS-CAT-CAU	3.83	123.00	117.36
3	C	402	COA	C4B-O4B-C1B	-3.71	106.53	109.92
3	B	402	COA	C6P-C5P-N4P	3.54	122.79	116.34
4	A	401	14U	CAB-CAU-CAE	-3.39	107.29	110.80
4	B	401	14U	CAR-CAS-CAT	-3.31	108.42	114.50
3	B	402	COA	C7P-C6P-C5P	-3.30	106.90	112.39
4	A	401	14U	CAS-CAT-CAU	2.87	121.59	117.36
3	B	402	COA	O5P-C5P-C6P	-2.69	117.14	122.02
3	B	402	COA	O5A-P2A-O6A	2.57	119.22	107.57
3	B	402	COA	O5A-P2A-O3A	-2.37	100.86	107.27
3	B	402	COA	CEP-CBP-CAP	2.36	112.80	108.77
4	A	401	14U	CAR-CAS-CAT	-2.30	110.27	114.50
3	C	402	COA	O6A-P2A-O4A	2.25	117.86	108.94
4	B	401	14U	OAD-CAT-CAU	-2.08	118.02	121.21
2	C	401	PLM	C4-C3-C2	2.08	120.75	113.13
3	C	402	COA	O5A-P2A-O6A	2.07	116.97	107.57
3	C	402	COA	O2A-P1A-O3A	2.04	112.79	107.27
4	A	401	14U	CAE-CAU-CAT	2.02	115.25	109.30

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	COA	CCP-O6A-P2A-O3A
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	B	402	COA	C5B-O5B-P1A-O1A
3	B	402	COA	C5B-O5B-P1A-O3A
3	B	402	COA	CCP-O6A-P2A-O3A
3	B	402	COA	CCP-O6A-P2A-O4A
3	B	402	COA	CDP-CBP-CCP-O6A
3	B	402	COA	CEP-CBP-CCP-O6A
3	B	402	COA	CAP-CBP-CCP-O6A
3	B	402	COA	S1P-C2P-C3P-N4P
4	B	401	14U	OAC-CAE-CAU-CAT
4	A	401	14U	OAC-CAE-CAU-CAB
4	A	401	14U	OAC-CAE-CAU-CAT

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Mol	Chain	Res	Type	Atoms
3	C	402	COA	C3B-C4B-C5B-O5B
3	C	402	COA	O4B-C4B-C5B-O5B
3	B	402	COA	C5P-C6P-C7P-N8P
3	C	402	COA	C5B-O5B-P1A-O1A
3	C	402	COA	CCP-O6A-P2A-O4A
3	B	402	COA	C5B-O5B-P1A-O2A
3	C	402	COA	C5P-C6P-C7P-N8P
2	D	401	PLM	O1-C1-C2-C3
2	D	401	PLM	O2-C1-C2-C3
4	B	401	14U	OAD-CAT-CAU-CAE

There are no ring outliers.

6 monomers are involved in 21 short contacts:

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

Bond lengths

Bond angles

Torsions

Rings

Ligand PLM C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand PLM D 401

Bond lengths

Bond angles

Torsions

Rings

Ligand 14U B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand COA C 402

Bond lengths

Bond angles

Torsions

Rings

Ligand 14U A 401

Bond lengths

Bond angles

Torsions

Rings
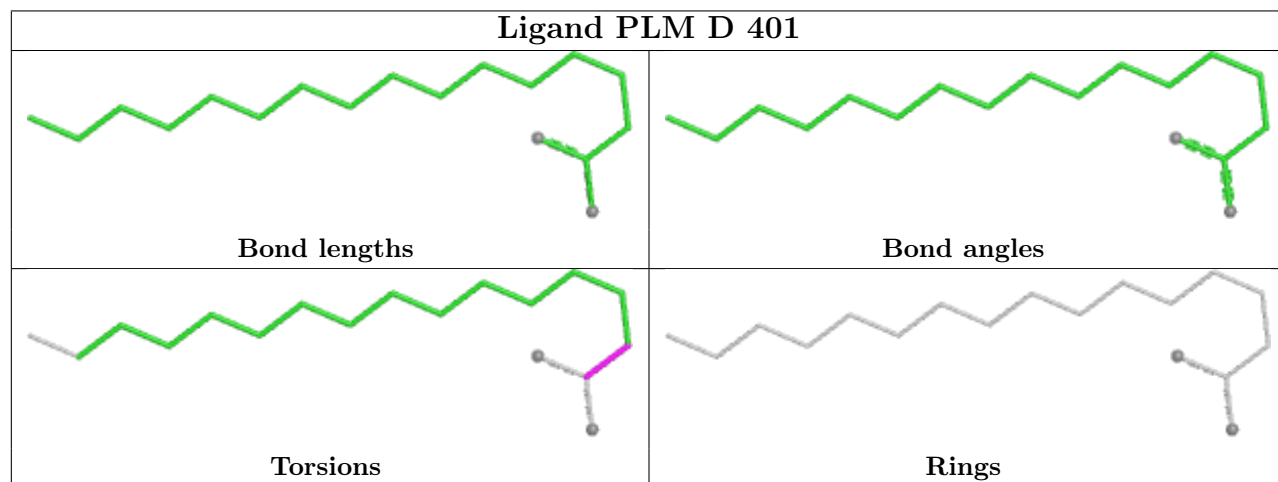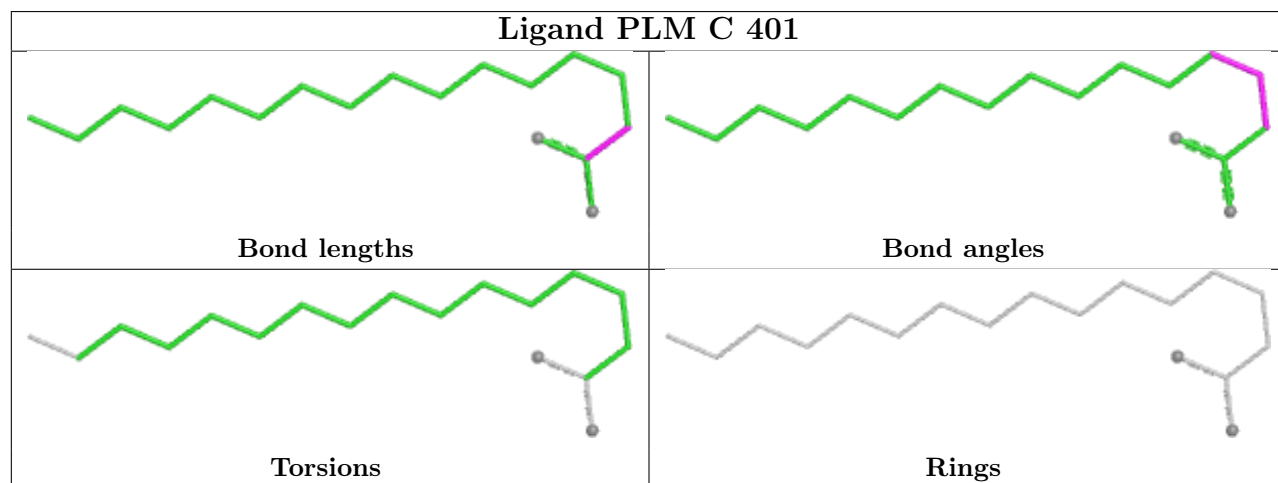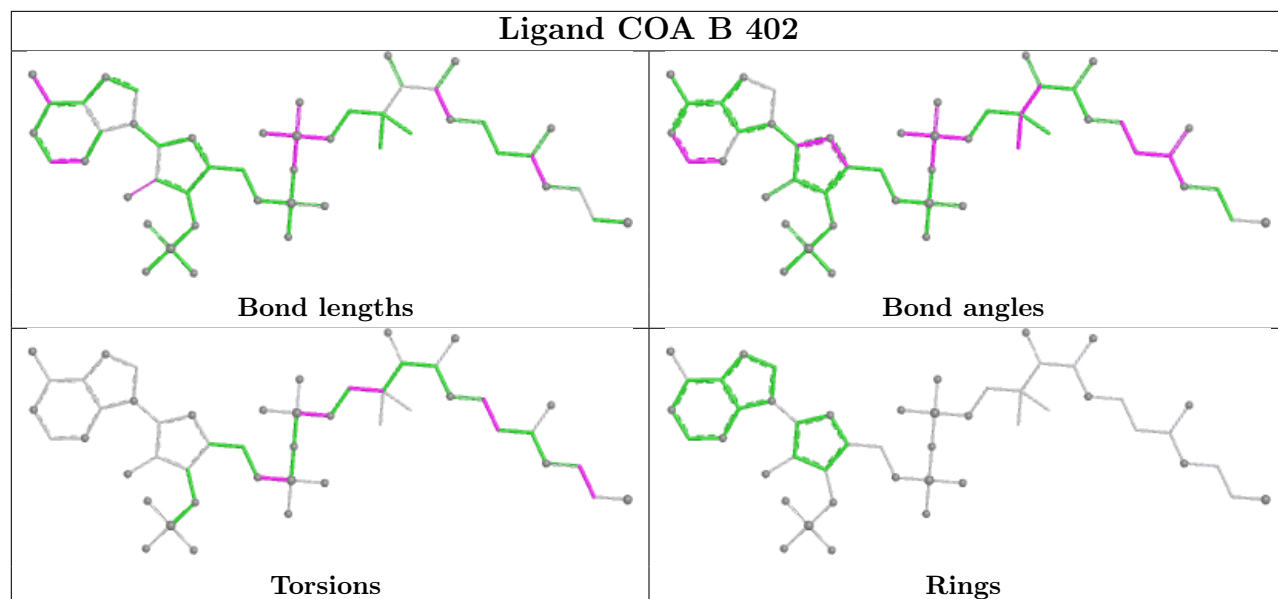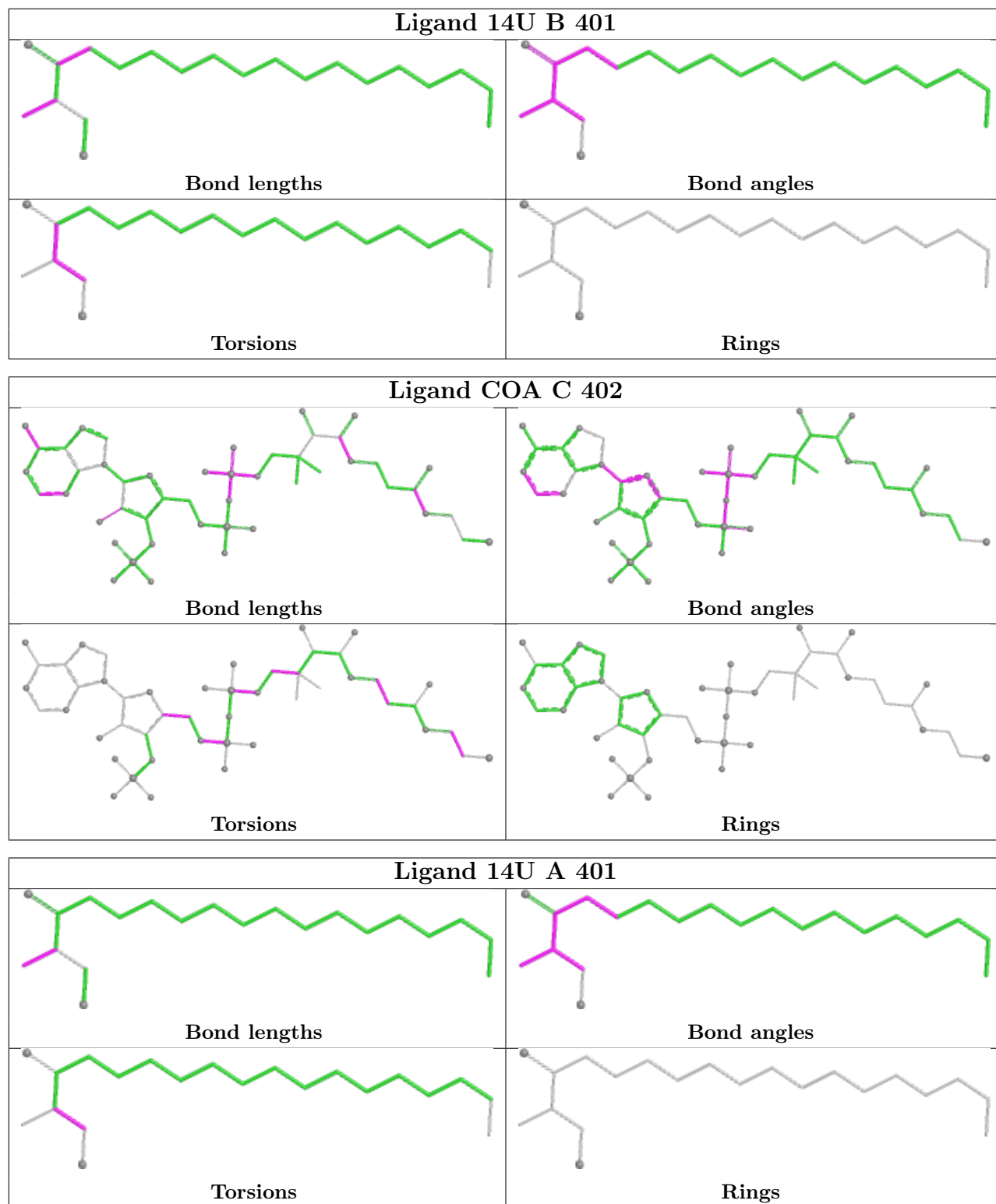
5.7 Other polymers ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	353/353 (100%)	0.45	8 (2%)	61	66	35, 51, 69, 80	0
1	B	352/353 (99%)	0.23	4 (1%)	77	84	31, 47, 66, 76	0
1	C	353/353 (100%)	0.37	2 (0%)	85	91	38, 55, 71, 79	0
1	D	352/353 (99%)	0.43	7 (1%)	64	71	38, 56, 71, 81	0
All	All	1410/1412 (99%)	0.37	21 (1%)	71	79	31, 53, 71, 81	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	3.2
1	D	352	TRP	3.2
1	A	252	TYR	3.1
1	D	31	LEU	3.0
1	A	208	ALA	2.9
1	B	252	TYR	2.7
1	B	279	GLY	2.6
1	A	1	MET	2.6
1	A	210	GLY	2.6
1	A	279	GLY	2.6
1	B	295	PRO	2.4
1	D	294	PRO	2.3
1	A	206	VAL	2.3
1	D	45	ALA	2.2
1	D	353	ARG	2.2
1	D	297	ALA	2.2
1	B	296	GLU	2.2
1	D	275	VAL	2.1
1	C	206	VAL	2.1
1	A	264	HIS	2.1
1	A	271	ILE	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 monosaccharides 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
3	COA	C	402	48/48	0.73	0.13	61,76,88,94	0
2	PLM	C	401	18/18	0.83	0.15	51,55,66,67	0
4	14U	B	401	21/22	0.85	0.14	37,44,56,62	0
3	COA	B	402	48/48	0.86	0.10	47,62,71,75	0
2	PLM	D	401	18/18	0.90	0.13	53,59,66,68	0
4	14U	A	401	21/22	0.90	0.14	38,47,53,54	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 COA 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)
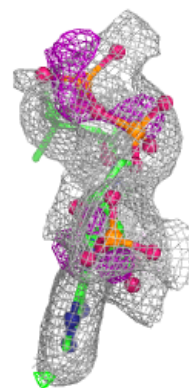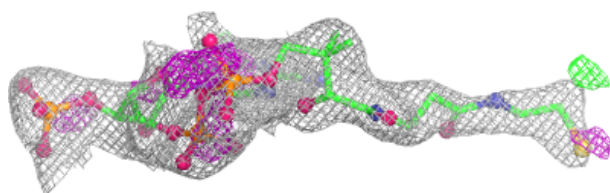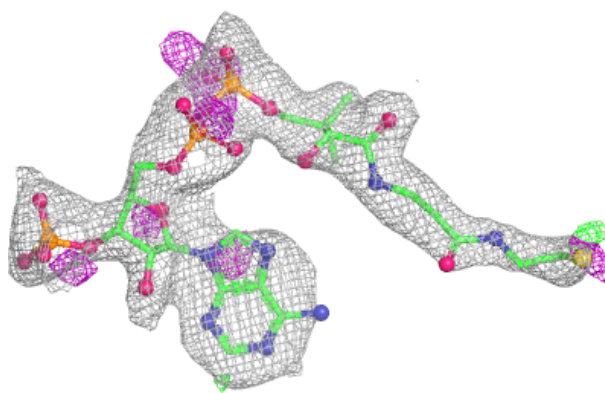
Electron density around PLM C 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
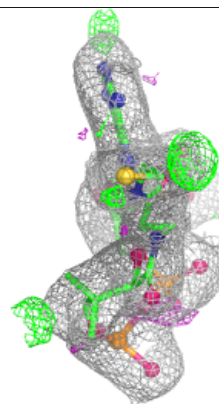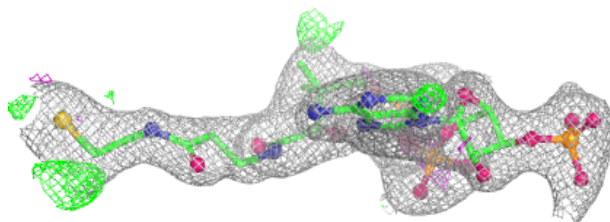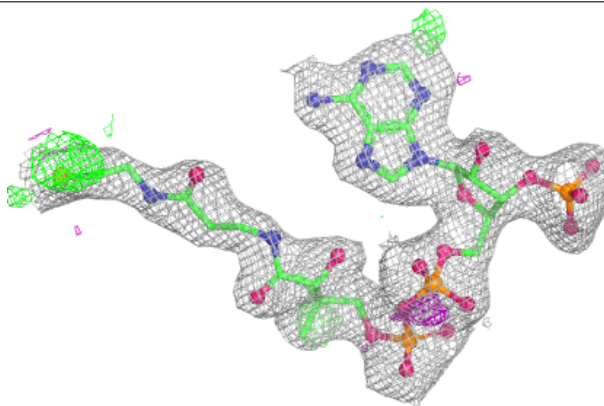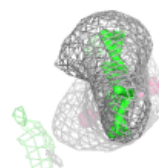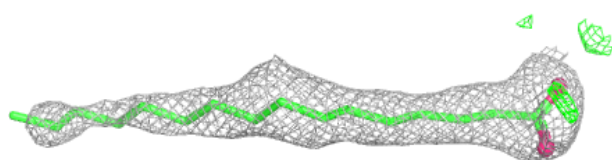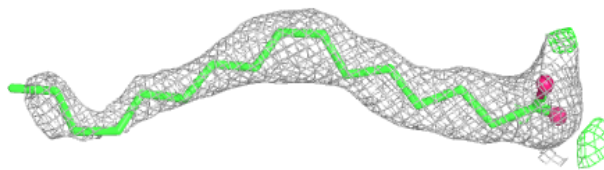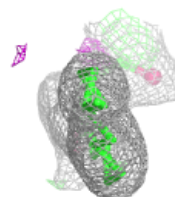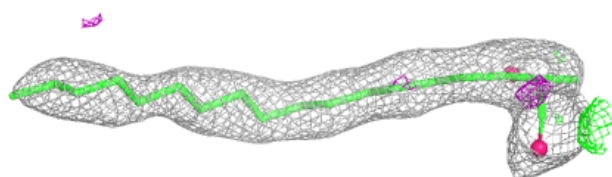mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
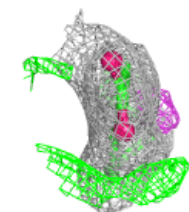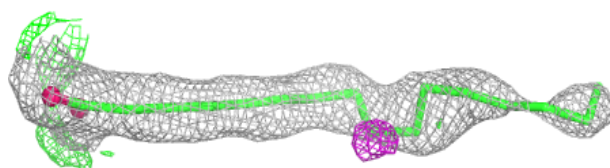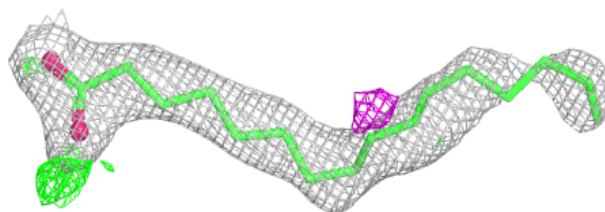
Electron density around 14U B 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
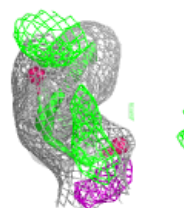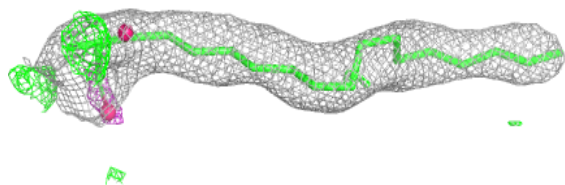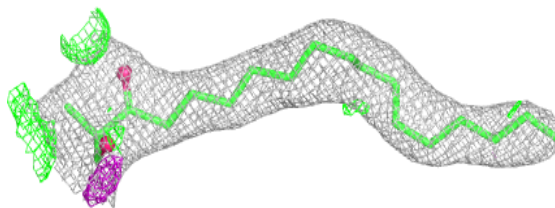
Electron density around COA B 402:

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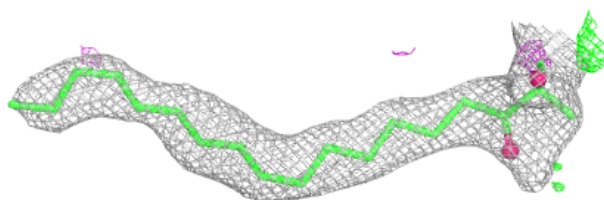$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around PLM 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 14U 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.