Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:06 AM EDT

PDB ID	:	2I79
Title	:	The crystal structure of the acetyltransferase of GNAT family from Streptococcus pneumoniae
Authors	:	Zhang, R.G.; Zhou, M.; Abdullah, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2006-08-30
Resolution	:	2.10 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

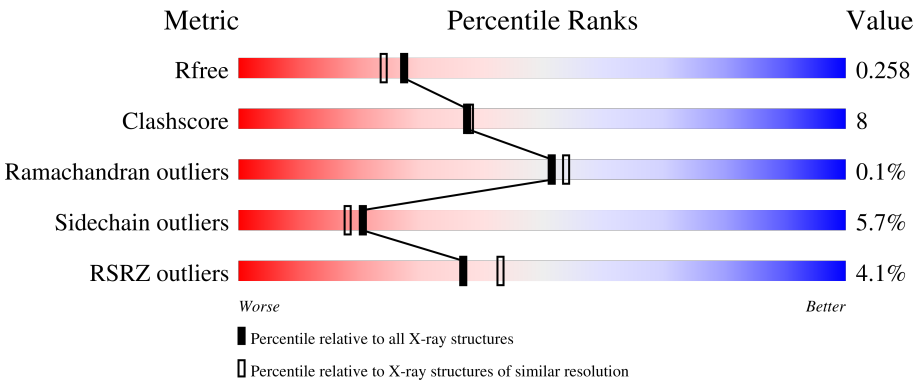
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	172	3% 77% 21% •••
1	B	172	2% 80% 19% ••
1	C	172	3% 86% 12% •••
1	D	172	2% 83% 13% •• •

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Mol	Chain	Length	Quality of chain
1	E	172	9% 77% 19%
1	F	172	3% 77% 17%

2 Entry composition (i)

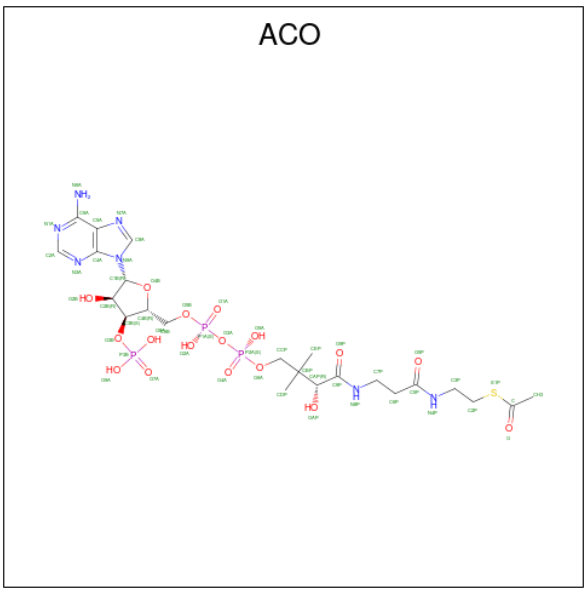
There are 3 unique types of molecules in this entry. The entry contains 8706 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetyltransferase, GNAT family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	171	1359	866	234	256	3	0	0	0
			Total	C	N	O	S			
1	B	171	1359	866	234	256	3	0	0	0
			Total	C	N	O	S			
1	C	171	1359	866	234	256	3	0	0	0
			Total	C	N	O	S			
1	D	167	1321	842	230	247	2	0	0	0
			Total	C	N	O	S			
1	E	168	1330	847	231	250	2	0	0	0
			Total	C	N	O	S			
1	F	168	1333	851	231	249	2	0	0	0

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	51	23	7	17	3	1	0	0
2	B	1	51	23	7	17	3	1	0	0
2	C	1	51	23	7	17	3	1	0	0
2	D	1	51	23	7	17	3	1	0	0
2	E	1	51	23	7	17	3	1	0	0
2	F	1	51	23	7	17	3	1	0	0

- Molecule 3 is water.

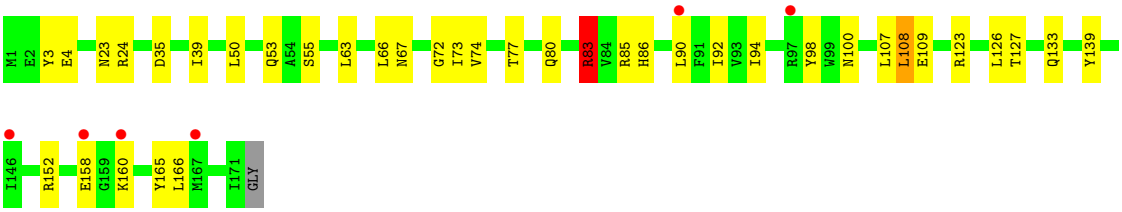
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	62	62	62	0	0
3	B	56	56	56	0	0
3	C	50	50	50	0	0
3	D	74	74	74	0	0
3	E	57	57	57	0	0
3	F	40	40	40	0	0

3 Residue-property plots (i)

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.

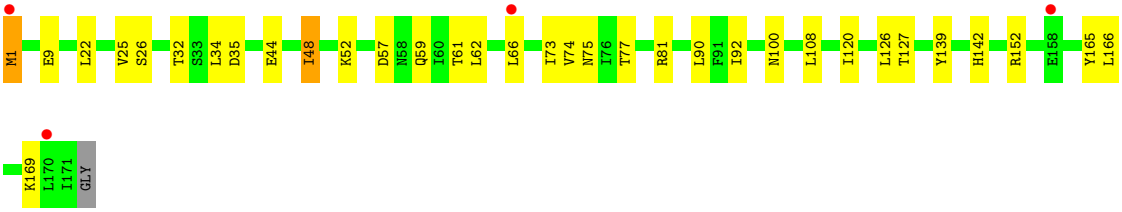
• Molecule 1: Acetyltransferase, GNAT family

Chain A:



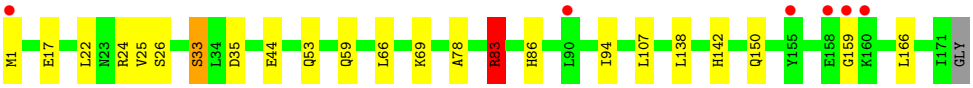
• Molecule 1: Acetyltransferase, GNAT family

Chain B:



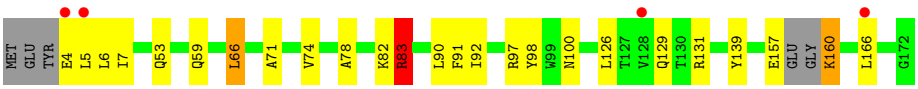
• Molecule 1: Acetyltransferase, GNAT family

Chain C:



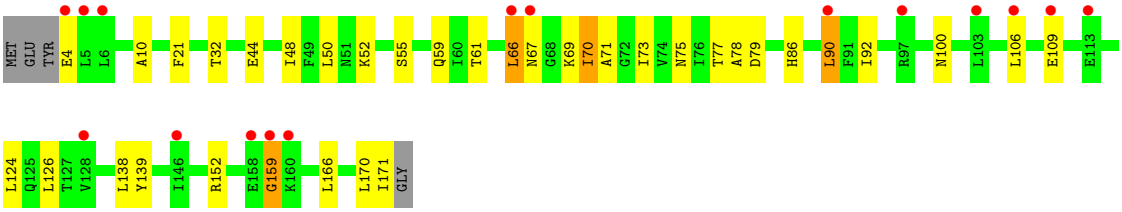
• Molecule 1: Acetyltransferase, GNAT family

Chain D:



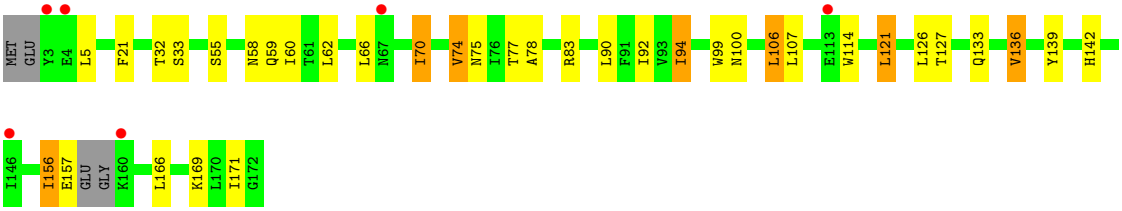
• Molecule 1: Acetyltransferase, GNAT family

Chain E:



- Molecule 1: Acetyltransferase, GNAT family

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	133.13Å 174.79Å 56.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.70 – 2.10 44.73 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.5 (44.70-2.10) 93.5 (44.73-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.97 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.251 0.215 , 0.258	Depositor DCC
R_{free} test set	3647 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	41.2	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8706	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACO

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	0.73	0/1378	0.88	6/1857 (0.3%)
1	B	0.68	0/1378	0.76	1/1857 (0.1%)
1	C	0.66	0/1378	0.81	2/1857 (0.1%)
1	D	0.69	0/1338	0.78	2/1802 (0.1%)
1	E	0.65	0/1348	0.76	1/1817 (0.1%)
1	F	0.66	0/1351	0.80	1/1820 (0.1%)
All	All	0.68	0/8171	0.80	13/11010 (0.1%)

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	E	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	83	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	A	123	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	A	123	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	C	83	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	A	24	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	A	83	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	D	83	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	D	83	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	83	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	E	159	GLY	N-CA-C	-6.31	97.32	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	35	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	35	ASP	CB-CG-OD1	5.46	123.22	118.30
1	F	83	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	159	GLY	Peptide

5.2 Too-close contacts (i)

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	1359	0	1378	26	0
1	B	1359	0	1378	23	0
1	C	1359	0	1378	16	0
1	D	1321	0	1344	32	0
1	E	1330	0	1351	23	0
1	F	1333	0	1353	24	0
2	A	51	0	34	2	0
2	B	51	0	34	4	0
2	C	51	0	34	0	0
2	D	51	0	34	10	0
2	E	51	0	34	1	0
2	F	51	0	34	2	0
3	A	62	0	0	1	0
3	B	56	0	0	1	0
3	C	50	0	0	4	0
3	D	74	0	0	6	0
3	E	57	0	0	2	0
3	F	40	0	0	1	0
All	All	8706	0	8386	129	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 8.

All (129) 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:166:LEU:CD1	1:F:166:LEU:HD13	1.79	1.12
1:D:166:LEU:HD13	1:F:166:LEU:CD1	1.80	1.08
1:D:91:PHE:CD1	2:D:404:ACO:HH32	1.89	1.06
1:B:166:LEU:HD13	1:C:166:LEU:HD13	1.47	0.93
1:D:92:ILE:N	2:D:404:ACO:HH31	1.85	0.91
2:B:401:ACO:H62A	1:D:100:ASN:HD21	1.21	0.87
1:D:166:LEU:HD13	1:F:166:LEU:HD13	0.90	0.87
1:A:100:ASN:HD21	2:A:402:ACO:H8A	1.41	0.86
1:D:157:GLU:OE2	3:D:407:HOH:O	1.94	0.83
1:D:92:ILE:O	2:D:404:ACO:HH33	1.81	0.80
1:D:160:LYS:N	3:D:429:HOH:O	2.12	0.80
1:D:92:ILE:O	2:D:404:ACO:CH3	2.30	0.80
1:D:91:PHE:CE1	2:D:404:ACO:HH32	2.19	0.77
1:B:75:ASN:OD1	1:B:77:THR:HG23	1.85	0.75
1:B:100:ASN:HD21	2:B:401:ACO:H8A	1.51	0.74
1:D:4:GLU:N	3:D:439:HOH:O	2.21	0.73
1:F:92:ILE:HG22	1:F:139:TYR:OH	1.91	0.70
1:D:92:ILE:H	2:D:404:ACO:HH31	1.53	0.70
1:A:166:LEU:HD13	1:E:166:LEU:HD13	1.74	0.69
1:A:100:ASN:ND2	2:A:402:ACO:H8A	2.08	0.69
1:D:91:PHE:CD1	2:D:404:ACO:CH3	2.74	0.68
1:D:53:GLN:O	3:D:405:HOH:O	2.12	0.67
1:D:83:ARG:HD2	1:F:32:THR:O	1.95	0.67
1:B:1:MET:SD	1:B:1:MET:N	2.61	0.65
1:C:53:GLN:O	3:C:416:HOH:O	2.14	0.65
1:D:157:GLU:HB2	3:D:424:HOH:O	1.98	0.63
1:A:66:LEU:HD23	1:A:98:TYR:CD2	2.34	0.63
1:D:66:LEU:HD23	1:D:98:TYR:CD1	2.34	0.62
1:B:59:GLN:O	3:B:438:HOH:O	2.16	0.62
1:F:133:GLN:HA	1:F:136:VAL:HG13	1.82	0.61
1:E:90:LEU:HD11	1:E:124:LEU:HD13	1.81	0.61
1:A:158:GLU:O	1:A:158:GLU:HG2	2.00	0.61
1:C:59:GLN:HE21	1:C:78:ALA:H	1.49	0.60
1:F:106:LEU:HD13	3:F:426:HOH:O	2.02	0.59
1:F:142:HIS:O	1:F:169:LYS:HE2	2.03	0.58
1:A:83:ARG:HD2	1:E:32:THR:O	2.04	0.57
1:B:32:THR:O	1:C:83:ARG:HD2	2.04	0.57
1:A:90:LEU:HD21	1:A:108:LEU:HD21	1.86	0.57
1:F:74:VAL:HG22	1:F:107:LEU:HB3	1.87	0.56
1:F:90:LEU:O	2:F:406:ACO:HH31	2.06	0.56
1:F:127:THR:HG22	1:F:166:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLN:O	3:A:404:HOH:O	2.17	0.56
1:B:57:ASP:OD2	1:B:120:ILE:HD13	2.06	0.56
1:F:100:ASN:HD21	2:F:406:ACO:H8A	1.70	0.55
1:B:126:LEU:HD11	1:B:139:TYR:CE2	2.42	0.55
1:B:100:ASN:ND2	2:B:401:ACO:H8A	2.21	0.55
1:A:152:ARG:O	1:E:86:HIS:HE1	1.90	0.54
1:E:126:LEU:HD11	1:E:139:TYR:CE2	2.43	0.54
1:D:126:LEU:HD11	1:D:139:TYR:CE2	2.44	0.53
1:A:4:GLU:H	1:A:67:ASN:ND2	2.06	0.53
1:B:9:GLU:HA	1:B:62:LEU:HD23	1.90	0.52
1:D:129:GLN:NE2	1:D:131:ARG:HE	2.08	0.52
1:A:152:ARG:HD2	1:E:170:LEU:HD22	1.92	0.52
1:A:23:ASN:ND2	1:A:39:ILE:H	2.08	0.52
1:C:94:ILE:HD11	1:C:107:LEU:HD12	1.91	0.51
1:C:150:GLN:HG3	1:C:166:LEU:HD11	1.93	0.51
1:C:59:GLN:NE2	1:C:78:ALA:H	2.08	0.51
1:D:92:ILE:H	2:D:404:ACO:CH3	2.21	0.51
1:E:21:PHE:CD2	1:E:70:ILE:HD11	2.45	0.51
1:D:157:GLU:CD	3:D:407:HOH:O	2.44	0.51
1:A:127:THR:HG22	1:A:166:LEU:HD23	1.93	0.51
1:A:66:LEU:HD23	1:A:98:TYR:CE2	2.45	0.51
1:F:94:ILE:HD11	1:F:99:TRP:HA	1.92	0.50
1:B:142:HIS:O	1:B:169:LYS:HE3	2.12	0.50
1:C:17:GLU:HG3	3:C:410:HOH:O	2.10	0.50
1:B:48:ILE:O	1:B:52:LYS:HG2	2.12	0.50
1:D:92:ILE:O	2:D:404:ACO:HH31	2.10	0.50
1:D:74:VAL:HG23	1:D:92:ILE:HG12	1.92	0.50
1:C:59:GLN:O	3:C:416:HOH:O	2.19	0.49
1:B:166:LEU:CD1	1:C:166:LEU:HD13	2.32	0.49
1:F:21:PHE:CG	1:F:70:ILE:CD1	2.95	0.49
1:E:59:GLN:NE2	1:E:78:ALA:H	2.10	0.49
1:A:90:LEU:HD21	1:A:108:LEU:CD2	2.43	0.48
1:E:66:LEU:HD22	1:E:71:ALA:CB	2.44	0.48
1:D:71:ALA:HB1	1:D:98:TYR:CD2	2.49	0.48
1:B:26:SER:HB2	1:B:34:LEU:HB3	1.96	0.47
1:A:86:HIS:HE1	1:E:152:ARG:O	1.96	0.47
1:A:74:VAL:HG23	1:A:92:ILE:HG12	1.95	0.47
1:C:22:LEU:HA	1:C:25:VAL:HG22	1.96	0.47
1:A:72:GLY:HA3	1:A:94:ILE:HD13	1.96	0.46
1:B:90:LEU:O	2:B:401:ACO:HH31	2.15	0.46
1:E:124:LEU:HG	1:E:171:ILE:HD13	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:ILE:HG22	1:F:157:GLU:HG2	1.97	0.46
1:C:138:LEU:O	1:C:142:HIS:HD2	1.99	0.46
1:F:121:LEU:HB3	1:F:171:ILE:HD11	1.97	0.46
1:D:59:GLN:HE21	1:D:78:ALA:H	1.64	0.46
1:E:59:GLN:HE21	1:E:78:ALA:H	1.63	0.46
1:B:127:THR:HA	1:B:165:TYR:O	2.15	0.46
1:D:59:GLN:NE2	1:D:78:ALA:H	2.14	0.46
1:E:59:GLN:NE2	3:E:411:HOH:O	2.34	0.45
1:D:129:GLN:HE22	1:D:131:ARG:HH21	1.64	0.45
1:C:86:HIS:HD2	3:C:425:HOH:O	1.99	0.45
1:D:5:LEU:HD12	1:D:6:LEU:N	2.32	0.45
1:E:4:GLU:HB3	1:E:67:ASN:OD1	2.16	0.45
1:A:90:LEU:HD23	1:A:139:TYR:HE1	1.82	0.45
1:B:74:VAL:HG23	1:B:92:ILE:HG12	1.97	0.45
1:F:156:ILE:CG2	1:F:157:GLU:HG2	2.47	0.45
1:C:26:SER:HB3	1:C:35:ASP:O	2.17	0.45
1:F:75:ASN:OD1	1:F:77:THR:HG23	2.16	0.44
1:E:92:ILE:HG22	1:E:139:TYR:OH	2.17	0.44
1:D:5:LEU:HD11	1:D:7:ILE:HG13	1.98	0.44
1:F:60:ILE:HD12	1:F:114:TRP:CE2	2.52	0.44
1:E:61:THR:HG23	1:E:73:ILE:HD11	1.99	0.44
1:D:82:LYS:HA	1:D:82:LYS:HD3	1.84	0.44
1:F:62:LEU:HB2	1:F:74:VAL:HG23	2.00	0.44
1:B:44:GLU:O	1:B:48:ILE:HG23	2.18	0.43
1:D:92:ILE:H	2:D:404:ACO:C	2.31	0.43
1:E:10:ALA:CB	1:E:50:LEU:HD22	2.48	0.43
1:B:152:ARG:O	1:C:86:HIS:HE1	2.01	0.43
1:A:80:GLN:O	1:A:85:ARG:HD3	2.18	0.43
1:B:22:LEU:HA	1:B:25:VAL:HG22	2.00	0.43
1:E:86:HIS:HD2	3:E:418:HOH:O	2.01	0.43
1:E:59:GLN:HE21	1:E:77:THR:HA	1.83	0.43
1:F:60:ILE:HD12	1:F:114:TRP:NE1	2.34	0.42
1:E:100:ASN:OD1	2:E:405:ACO:H8A	2.19	0.42
1:A:166:LEU:CD1	1:E:166:LEU:HD13	2.48	0.42
1:B:61:THR:OG1	1:B:75:ASN:ND2	2.52	0.42
1:A:127:THR:HA	1:A:165:TYR:O	2.20	0.42
1:A:3:TYR:HA	1:A:67:ASN:HD21	1.86	0.41
1:E:48:ILE:O	1:E:52:LYS:HG3	2.21	0.41
1:E:90:LEU:CD1	1:E:124:LEU:HB3	2.49	0.41
1:F:21:PHE:CD1	1:F:70:ILE:HD13	2.55	0.41
1:A:63:LEU:CD2	1:A:73:ILE:HG22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ARG:HD3	1:C:33:SER:O	2.19	0.41
1:F:58:ASN:HB2	1:F:121:LEU:CD1	2.51	0.41
1:B:126:LEU:HD11	1:B:139:TYR:CZ	2.55	0.41
1:F:59:GLN:NE2	1:F:78:ALA:H	2.19	0.41
1:A:50:LEU:HD23	1:A:50:LEU:HA	1.94	0.40
1:A:126:LEU:HD11	1:A:139:TYR:CE2	2.56	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	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
1	B	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
1	C	169/172 (98%)	165 (98%)	3 (2%)	1 (1%)	25	21
1	D	163/172 (95%)	162 (99%)	1 (1%)	0	100	100
1	E	166/172 (96%)	162 (98%)	4 (2%)	0	100	100
1	F	164/172 (95%)	162 (99%)	2 (1%)	0	100	100
All	All	1000/1032 (97%)	982 (98%)	17 (2%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	159	GLY

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	143/143 (100%)	135 (94%)	8 (6%)	21	18
1	B	143/143 (100%)	138 (96%)	5 (4%)	36	38
1	C	143/143 (100%)	136 (95%)	7 (5%)	25	23
1	D	139/143 (97%)	134 (96%)	5 (4%)	35	36
1	E	140/143 (98%)	129 (92%)	11 (8%)	12	9
1	F	140/143 (98%)	128 (91%)	12 (9%)	10	7
All	All	848/858 (99%)	800 (94%)	48 (6%)	20	18

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	SER
1	A	77	THR
1	A	83	ARG
1	A	107	LEU
1	A	108	LEU
1	A	109	GLU
1	A	133	GLN
1	A	160	LYS
1	B	1	MET
1	B	48	ILE
1	B	66	LEU
1	B	73	ILE
1	B	108	LEU
1	C	1	MET
1	C	24	ARG
1	C	33	SER
1	C	44	GLU
1	C	66	LEU
1	C	69	LYS
1	C	83	ARG
1	D	66	LEU
1	D	83	ARG
1	D	90	LEU
1	D	97	ARG
1	D	160	LYS
1	E	44	GLU

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Mol	Chain	Res	Type
1	E	55	SER
1	E	66	LEU
1	E	69	LYS
1	E	70	ILE
1	E	75	ASN
1	E	79	ASP
1	E	90	LEU
1	E	106	LEU
1	E	109	GLU
1	E	138	LEU
1	F	5	LEU
1	F	33	SER
1	F	55	SER
1	F	66	LEU
1	F	70	ILE
1	F	74	VAL
1	F	94	ILE
1	F	106	LEU
1	F	121	LEU
1	F	126	LEU
1	F	136	VAL
1	F	156	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	59	GLN
1	A	67	ASN
1	A	75	ASN
1	A	80	GLN
1	A	86	HIS
1	A	100	ASN
1	B	80	GLN
1	B	100	ASN
1	C	59	GLN
1	C	75	ASN
1	C	86	HIS
1	C	142	HIS
1	D	59	GLN
1	D	75	ASN
1	D	100	ASN

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Mol	Chain	Res	Type
1	D	129	GLN
1	D	137	HIS
1	E	59	GLN
1	E	75	ASN
1	E	86	HIS
1	E	142	HIS
1	F	59	GLN
1	F	100	ASN
1	F	116	GLN

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 monosaccharides 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	$\#\|Z\| > 2$
2	ACO	C	403	-	47,53,53	1.39	3 (6%)	60,79,79	1.20	7 (11%)
2	ACO	B	401	-	47,53,53	0.92	3 (6%)	60,79,79	1.56	7 (11%)
2	ACO	A	402	-	47,53,53	1.12	3 (6%)	60,79,79	1.37	7 (11%)
2	ACO	F	406	-	47,53,53	1.07	4 (8%)	60,79,79	1.26	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACO	D	404	-	47,53,53	1.22	6 (12%)	60,79,79	1.24	9 (15%)
2	ACO	E	405	-	47,53,53	0.97	4 (8%)	60,79,79	1.28	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACO	C	403	-	-	9/47/67/67	0/3/3/3
2	ACO	B	401	-	-	6/47/67/67	0/3/3/3
2	ACO	A	402	-	-	6/47/67/67	0/3/3/3
2	ACO	F	406	-	-	6/47/67/67	0/3/3/3
2	ACO	D	404	-	-	4/47/67/67	0/3/3/3
2	ACO	E	405	-	-	4/47/67/67	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	403	ACO	P2A-O3A	5.47	1.65	1.59
2	C	403	ACO	P1A-O3A	4.61	1.64	1.59
2	A	402	ACO	P2A-O3A	4.36	1.64	1.59
2	F	406	ACO	P2A-O3A	3.42	1.63	1.59
2	D	404	ACO	P1A-O3A	3.35	1.63	1.59
2	C	403	ACO	O4B-C1B	3.11	1.45	1.40
2	E	405	ACO	P1A-O3A	3.00	1.62	1.59
2	F	406	ACO	P1A-O3A	2.83	1.62	1.59
2	D	404	ACO	C-S1P	-2.77	1.60	1.75
2	D	404	ACO	OAP-CAP	2.73	1.47	1.42
2	B	401	ACO	C-S1P	-2.67	1.60	1.75
2	E	405	ACO	P2A-O3A	2.67	1.62	1.59
2	A	402	ACO	P1A-O3A	2.64	1.62	1.59
2	D	404	ACO	P3B-O3B	2.58	1.64	1.59
2	B	401	ACO	P1A-O3A	2.37	1.62	1.59
2	D	404	ACO	O4B-C1B	2.36	1.44	1.40
2	E	405	ACO	O4B-C1B	2.30	1.43	1.40
2	A	402	ACO	C-S1P	-2.27	1.63	1.75
2	F	406	ACO	O4B-C1B	2.19	1.43	1.40
2	B	401	ACO	O4B-C4B	-2.07	1.40	1.45
2	F	406	ACO	C2A-N3A	2.02	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	405	ACO	C-S1P	-2.01	1.64	1.75
2	D	404	ACO	C5A-N7A	-2.01	1.32	1.39

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	ACO	N3A-C2A-N1A	-5.18	121.64	128.67
2	E	405	ACO	N3A-C2A-N1A	-4.78	122.19	128.67
2	B	401	ACO	C1B-N9A-C4A	-4.61	118.54	126.64
2	F	406	ACO	N3A-C2A-N1A	-4.54	122.50	128.67
2	A	402	ACO	N3A-C2A-N1A	-4.40	122.70	128.67
2	B	401	ACO	O3B-P3B-O7A	-3.92	95.35	109.33
2	C	403	ACO	C4A-C5A-N7A	-3.80	105.32	109.34
2	A	402	ACO	O3B-P3B-O7A	-3.76	95.92	109.33
2	E	405	ACO	O3B-P3B-O7A	-3.60	96.49	109.33
2	D	404	ACO	N3A-C2A-N1A	-3.57	123.82	128.67
2	A	402	ACO	C1B-N9A-C4A	-3.57	120.37	126.64
2	C	403	ACO	N3A-C2A-N1A	-3.28	124.22	128.67
2	D	404	ACO	O2A-P1A-O3A	3.08	115.59	107.27
2	F	406	ACO	C4A-C5A-N7A	-3.06	106.11	109.34
2	F	406	ACO	C1B-N9A-C4A	-2.98	121.40	126.64
2	D	404	ACO	O3B-P3B-O7A	-2.98	98.72	109.33
2	E	405	ACO	C1B-N9A-C4A	-2.89	121.56	126.64
2	B	401	ACO	O-C-S1P	-2.84	111.17	122.65
2	D	404	ACO	C4A-C5A-N7A	-2.65	106.54	109.34
2	A	402	ACO	O-C-S1P	-2.61	112.09	122.65
2	C	403	ACO	C2P-S1P-C	2.52	113.54	101.42
2	B	401	ACO	O5A-P2A-O4A	2.51	124.14	112.44
2	B	401	ACO	O-C-CH3	2.49	132.77	123.12
2	E	405	ACO	C4A-C5A-N7A	-2.49	106.70	109.34
2	D	404	ACO	N6A-C6A-N1A	2.48	123.64	118.33
2	C	403	ACO	C1B-N9A-C4A	-2.48	122.28	126.64
2	E	405	ACO	O5A-P2A-O4A	2.46	123.87	112.44
2	D	404	ACO	O4B-C1B-N9A	-2.44	105.50	108.75
2	F	406	ACO	C2P-S1P-C	2.42	113.08	101.42
2	C	403	ACO	C5A-C6A-N6A	2.30	123.81	120.31
2	C	403	ACO	O5A-P2A-O4A	2.28	123.03	112.44
2	D	404	ACO	CEP-CBP-CAP	2.24	112.58	108.77
2	A	402	ACO	C2P-S1P-C	2.23	112.14	101.42
2	E	405	ACO	O-C-S1P	-2.22	113.69	122.65
2	F	406	ACO	O4B-C1B-N9A	2.18	111.64	108.75
2	A	402	ACO	C4A-C5A-N7A	-2.17	107.05	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	404	ACO	C2P-S1P-C	2.13	111.64	101.42
2	B	401	ACO	C2P-S1P-C	2.12	111.60	101.42
2	A	402	ACO	O2A-P1A-O3A	2.09	112.93	107.27
2	C	403	ACO	O9A-P3B-O8A	2.08	115.61	107.80
2	F	406	ACO	O9A-P3B-O8A	2.06	115.54	107.80
2	F	406	ACO	O5A-P2A-O4A	2.05	121.99	112.44
2	D	404	ACO	O5A-P2A-O4A	2.00	121.76	112.44

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	ACO	O-C-S1P-C2P
2	A	402	ACO	CH3-C-S1P-C2P
2	B	401	ACO	O-C-S1P-C2P
2	B	401	ACO	CH3-C-S1P-C2P
2	C	403	ACO	O-C-S1P-C2P
2	C	403	ACO	CH3-C-S1P-C2P
2	D	404	ACO	C3P-C2P-S1P-C
2	D	404	ACO	O-C-S1P-C2P
2	D	404	ACO	CH3-C-S1P-C2P
2	E	405	ACO	O-C-S1P-C2P
2	E	405	ACO	CH3-C-S1P-C2P
2	F	406	ACO	C5B-O5B-P1A-O1A
2	F	406	ACO	O-C-S1P-C2P
2	F	406	ACO	CH3-C-S1P-C2P
2	B	401	ACO	C5P-C6P-C7P-N8P
2	A	402	ACO	O4B-C4B-C5B-O5B
2	A	402	ACO	C3B-C4B-C5B-O5B
2	C	403	ACO	C2B-C3B-O3B-P3B
2	C	403	ACO	C4B-C3B-O3B-P3B
2	C	403	ACO	C5B-O5B-P1A-O1A
2	D	404	ACO	C5B-O5B-P1A-O1A
2	E	405	ACO	C5B-O5B-P1A-O1A
2	F	406	ACO	C5B-O5B-P1A-O3A
2	F	406	ACO	C3B-O3B-P3B-O8A
2	A	402	ACO	C6P-C7P-N8P-C9P
2	C	403	ACO	O4B-C4B-C5B-O5B
2	C	403	ACO	C5P-C6P-C7P-N8P
2	F	406	ACO	C5P-C6P-C7P-N8P
2	B	401	ACO	O4B-C4B-C5B-O5B
2	E	405	ACO	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	C	403	ACO	C3B-O3B-P3B-O8A
2	B	401	ACO	C3B-C4B-C5B-O5B
2	C	403	ACO	C3B-C4B-C5B-O5B
2	A	402	ACO	P2A-O3A-P1A-O2A
2	B	401	ACO	P2A-O3A-P1A-O2A

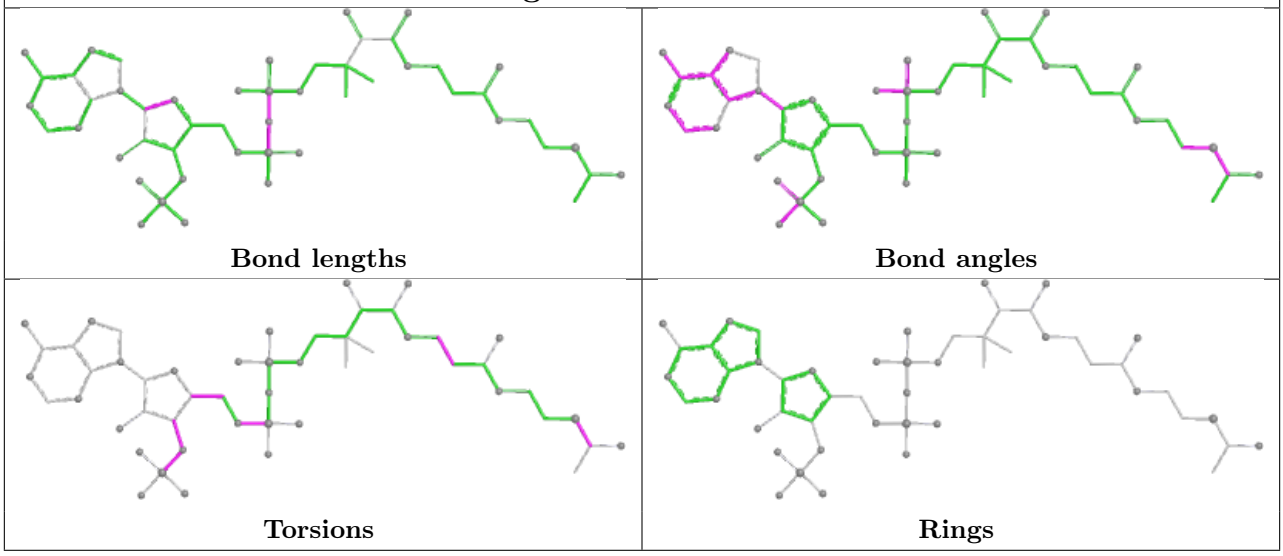
There are no ring outliers.

5 monomers are involved in 19 short contacts:

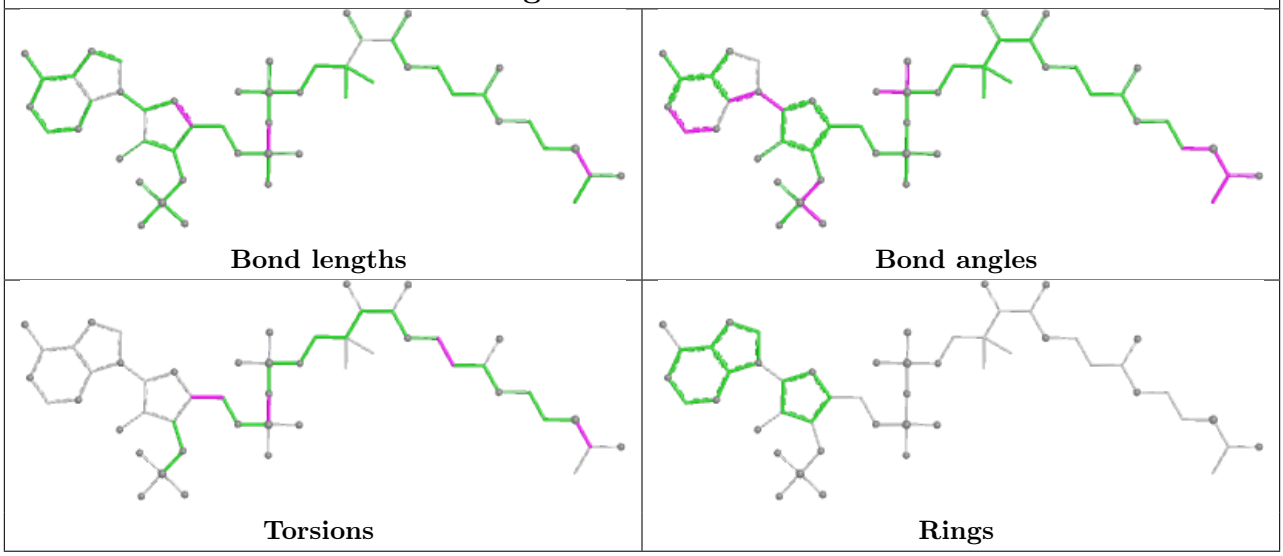
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	ACO	4	0
2	A	402	ACO	2	0
2	F	406	ACO	2	0
2	D	404	ACO	10	0
2	E	405	ACO	1	0

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.

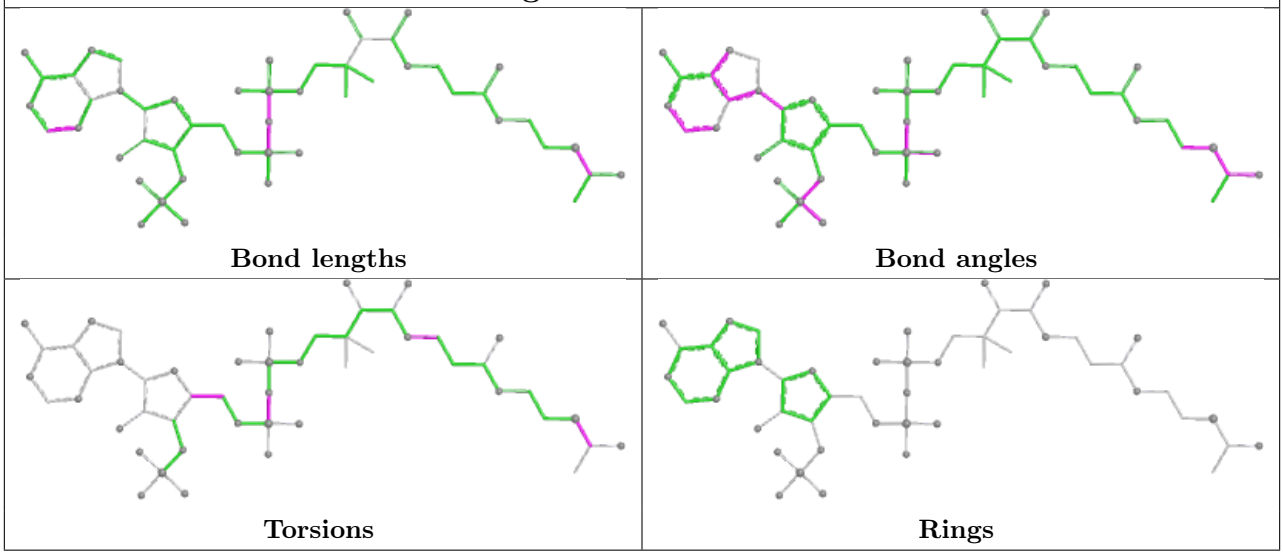
Ligand ACO C 403



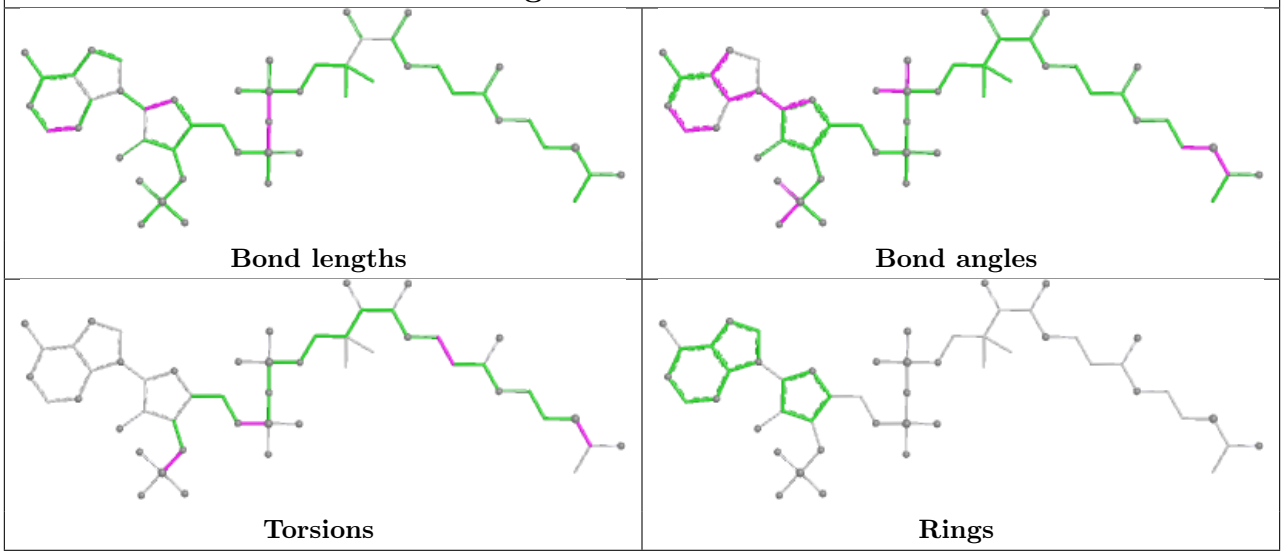
Ligand ACO B 401



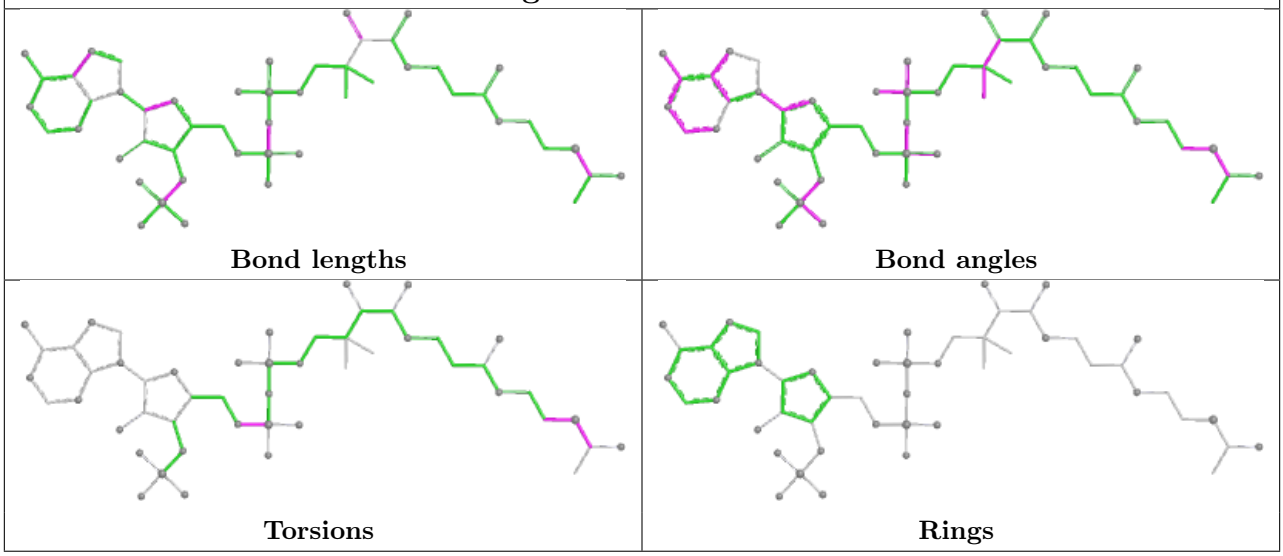
Ligand ACO A 402



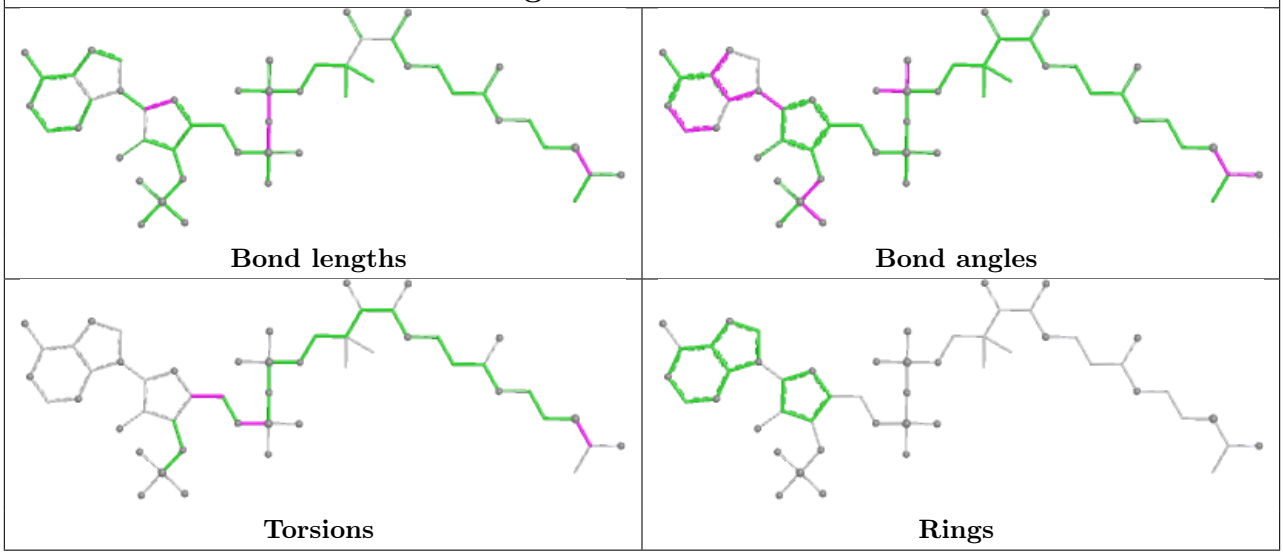
Ligand ACO F 406



Ligand ACO D 404



Ligand ACO E 405



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	171/172 (99%)	0.54	6 (3%)	44	50	39, 47, 62, 67	0
1	B	171/172 (99%)	0.49	4 (2%)	60	65	42, 48, 60, 73	0
1	C	171/172 (99%)	0.41	6 (3%)	44	50	38, 48, 56, 67	0
1	D	167/172 (97%)	0.57	4 (2%)	59	64	38, 47, 59, 71	0
1	E	168/172 (97%)	0.68	16 (9%)	8	10	40, 51, 61, 70	0
1	F	168/172 (97%)	0.56	6 (3%)	42	49	37, 46, 54, 69	0
All	All	1016/1032 (98%)	0.54	42 (4%)	37	43	37, 48, 60, 73	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	158	GLU	4.9
1	F	3	TYR	4.3
1	C	158	GLU	4.2
1	C	1	MET	4.2
1	B	158	GLU	4.1
1	E	4	GLU	3.8
1	E	159	GLY	3.6
1	A	158	GLU	3.4
1	E	146	ILE	3.2
1	E	5	LEU	3.1
1	B	170	LEU	3.0
1	F	160	LYS	2.8
1	B	1	MET	2.8
1	E	6	LEU	2.8
1	A	146	ILE	2.7
1	E	67	ASN	2.6
1	C	155	TYR	2.6
1	E	113	GLU	2.6
1	A	167	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	90	LEU	2.5
1	A	160	LYS	2.5
1	D	166	LEU	2.4
1	B	66	LEU	2.3
1	D	4	GLU	2.3
1	F	67	ASN	2.3
1	A	97	ARG	2.3
1	E	160	LYS	2.3
1	C	159	GLY	2.2
1	D	5	LEU	2.2
1	E	66	LEU	2.2
1	F	4	GLU	2.2
1	A	90	LEU	2.2
1	F	146	ILE	2.1
1	E	106	LEU	2.1
1	C	160	LYS	2.1
1	D	128	VAL	2.1
1	E	128	VAL	2.1
1	F	113	GLU	2.0
1	E	90	LEU	2.0
1	E	97	ARG	2.0
1	E	103	LEU	2.0
1	E	109	GLU	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.

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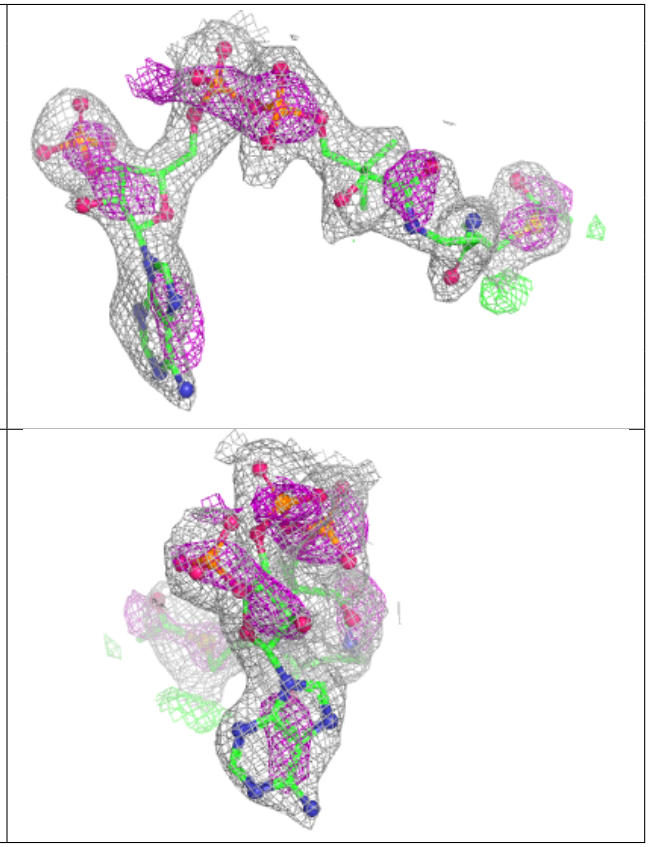
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACO	C	403	51/51	0.91	0.28	53,68,80,82	0
2	ACO	F	406	51/51	0.92	0.16	48,64,79,81	0
2	ACO	E	405	51/51	0.95	0.12	42,56,65,68	0
2	ACO	A	402	51/51	0.95	0.10	39,46,58,60	0
2	ACO	B	401	51/51	0.96	0.10	34,38,55,56	0
2	ACO	D	404	51/51	0.96	0.10	33,42,57,60	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.

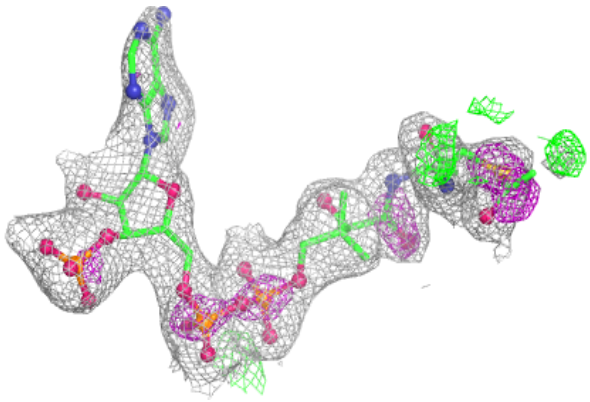
Electron density around ACO C 403:

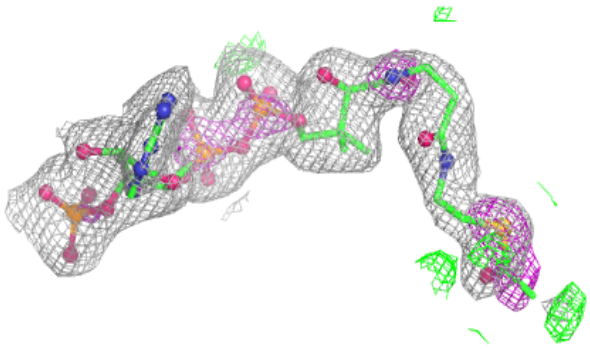
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

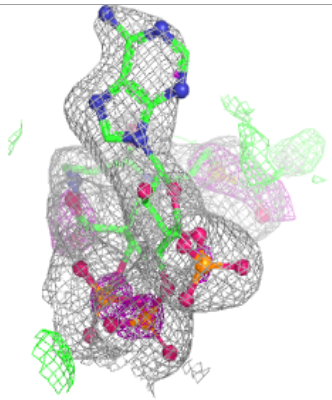


Electron density around ACO F 406:

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

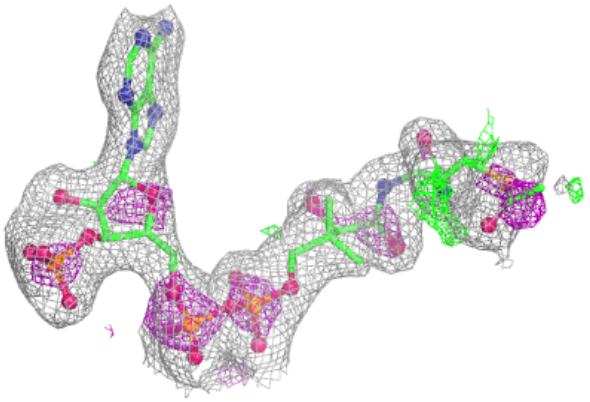


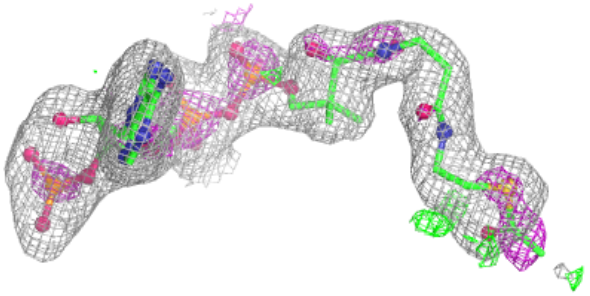


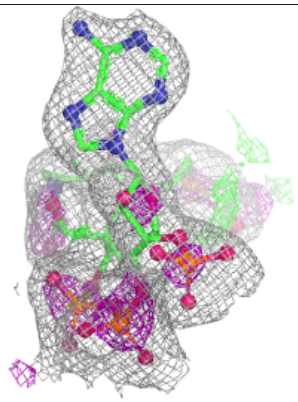


Electron density around ACO E 405:

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

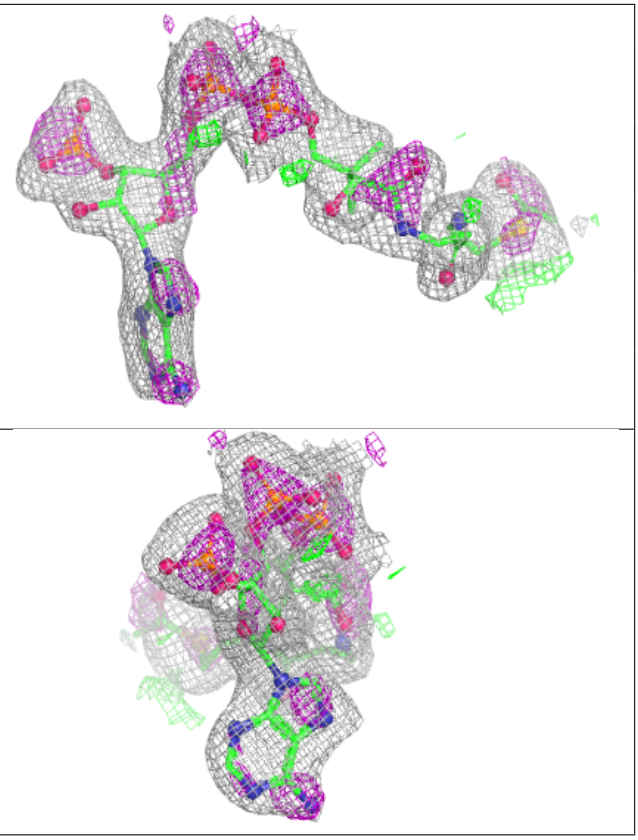






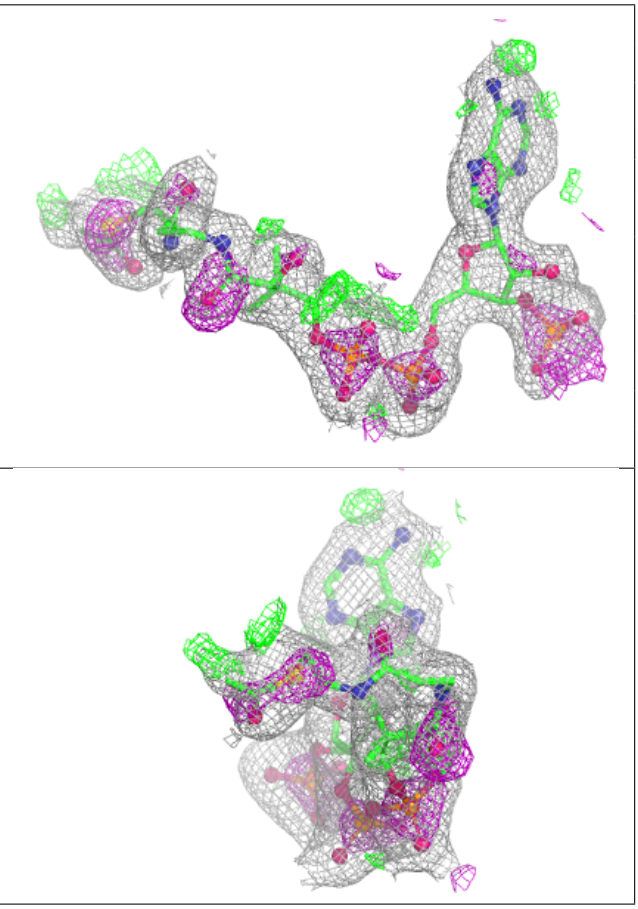
Electron density around ACO A 402:

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



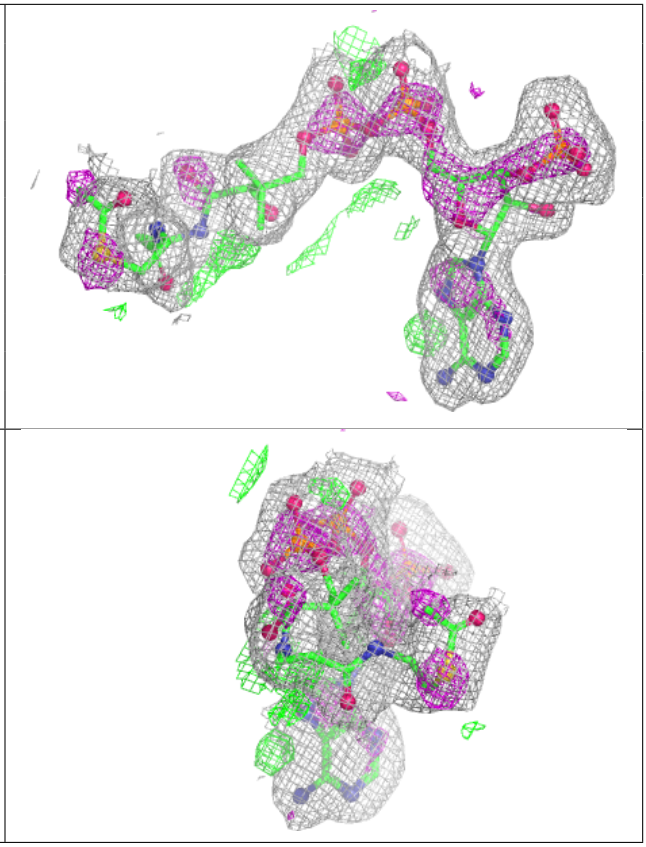
Electron density around ACO B 401:

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



Electron density around ACO D 404:

$2mF_o$-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.