



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:29 pm BST

PDB ID : 2GD6  
Title : The 1,1-proton transfer reaction mechanism by alpha-methylacyl-CoA race-  
mase is catalyzed by an aspartate/histidine pair and involves a smooth,  
methionine-rich surface for binding the fatty acyl moiety  
Authors : Bhaumik, P.; Wierenga, R.K.  
Deposited on : 2006-03-15  
Resolution : 2.30 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](mailto: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.

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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

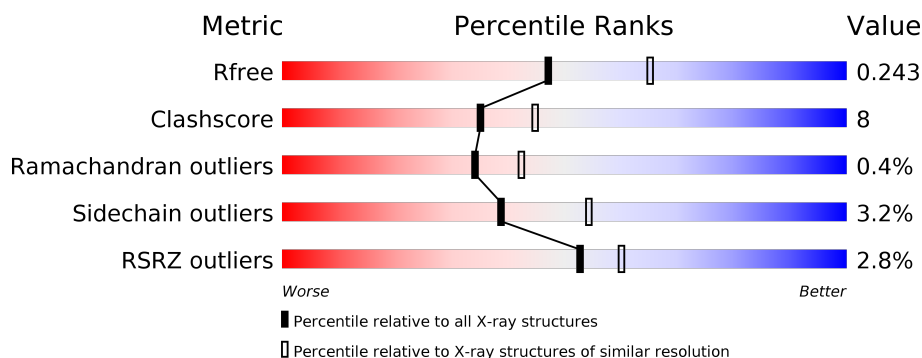
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	360	<div> <div>0%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>
1	B	360	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>
1	C	360	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>..</div> </div> </div>
1	D	360	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>..</div> </div> </div>

## 2 Entry composition [i](#)

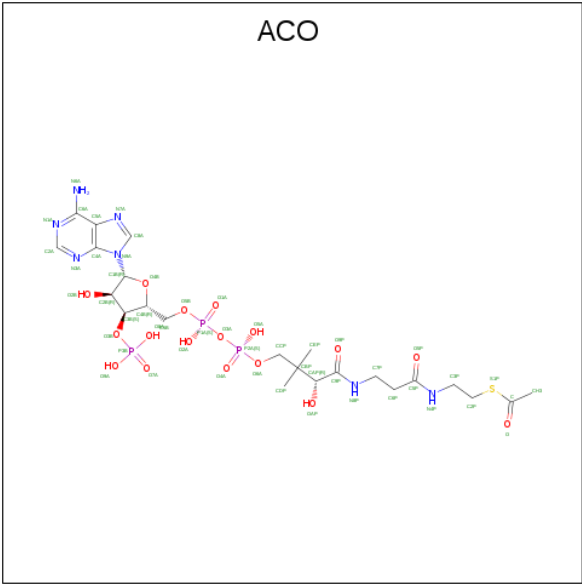
There are 4 unique types of molecules in this entry. The entry contains 11648 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 probable alpha-methylacyl-CoA racemase MCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	7	0
			2704	1694	488	506	16			
1	B	354	Total	C	N	O	S	0	4	0
			2696	1691	487	502	16			
1	C	354	Total	C	N	O	S	0	1	0
			2680	1683	481	501	15			
1	D	354	Total	C	N	O	S	0	1	0
			2680	1683	481	501	15			

- Molecule 2 is ACETYL COENZYME \*A (three-letter code: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



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

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

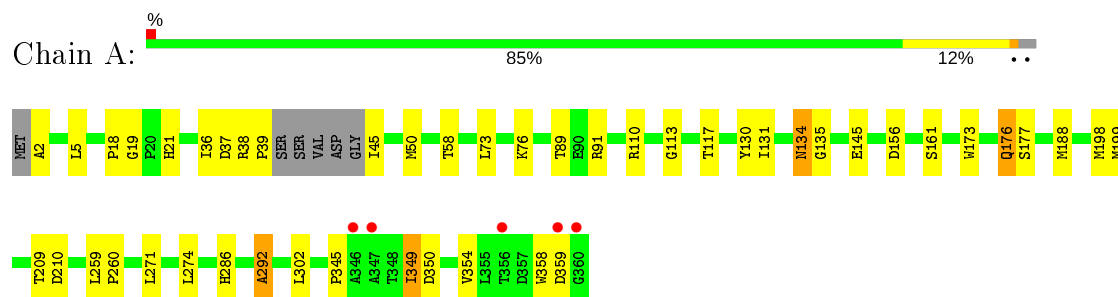
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	171	Total	O	0	0
			171	171		
4	B	185	Total	O	0	0
			185	185		
4	C	143	Total	O	0	0
			143	143		
4	D	173	Total	O	0	0
			173	173		

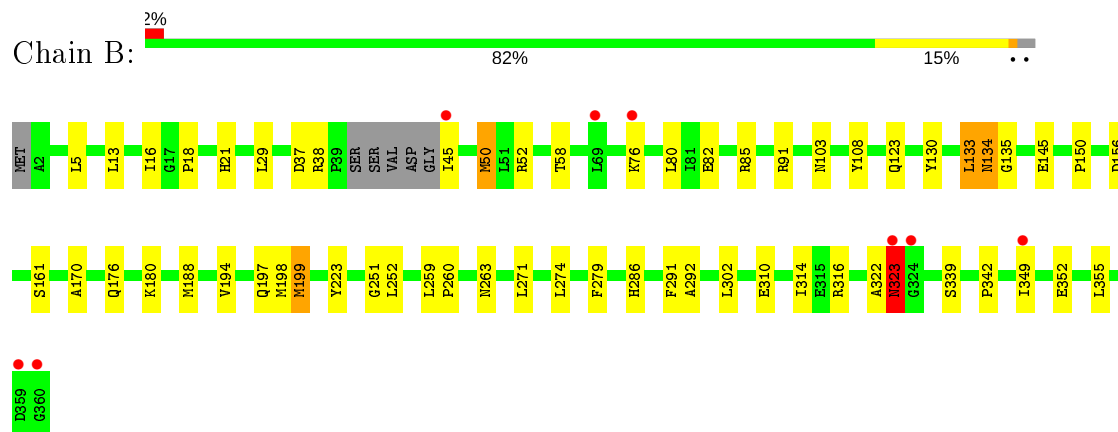
### 3 Residue-property plots [i](#)

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.

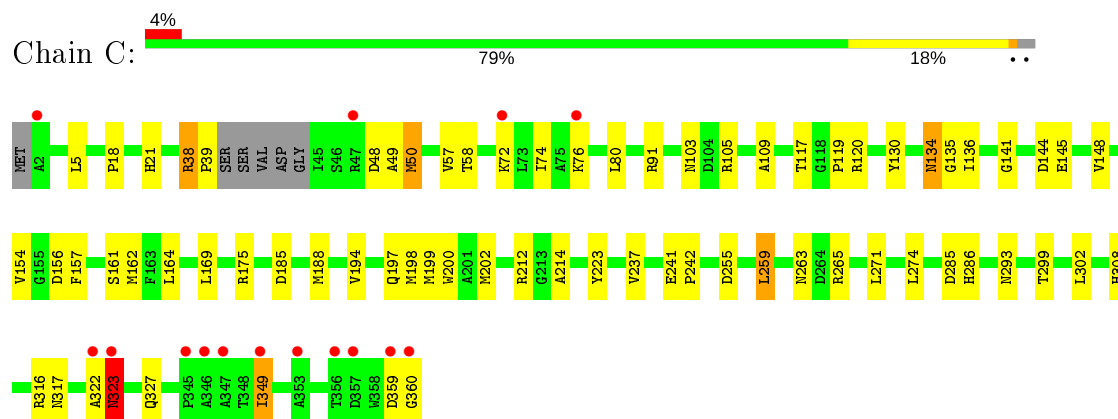
- Molecule 1: probable alpha-methylacyl-CoA racemase MCR



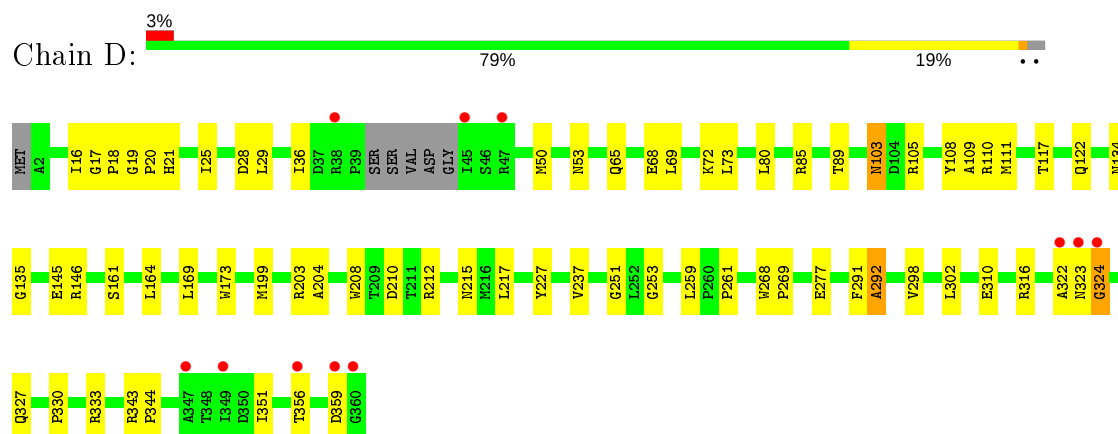
- Molecule 1: probable alpha-methylacyl-CoA racemase MCR



- Molecule 1: probable alpha-methylacyl-CoA racemase MCR



- Molecule 1: probable alpha-methylacyl-CoA racemase MCR



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.91Å 79.94Å 118.39Å 90.00° 91.03° 90.00°	Depositor
Resolution (Å)	19.71 – 2.30 19.71 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.71-2.30) 93.9 (19.71-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.98 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.219 , 0.270 0.224 , 0.243	Depositor DCC
$R_{free}$ test set	3713 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.327 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11648	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7998e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: GOL, 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	0.61	0/2801	0.69	0/3807
1	B	0.61	0/2778	0.70	1/3776 (0.0%)
1	C	0.57	0/2746	0.67	1/3735 (0.0%)
1	D	0.57	0/2746	0.66	0/3735
All	All	0.59	0/11071	0.68	2/15053 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	LEU	CA-CB-CG	5.92	128.91	115.30
1	C	259	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2704	0	2639	38	0
1	B	2696	0	2638	43	0
1	C	2680	0	2624	58	0
1	D	2680	0	2624	56	0
2	A	51	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	51	0	34	3	0
2	C	51	0	34	9	0
2	D	51	0	34	2	0
3	A	6	0	8	2	0
3	C	6	0	8	0	0
4	A	171	0	0	10	0
4	B	185	0	0	8	0
4	C	143	0	0	15	0
4	D	173	0	0	15	0
All	All	11648	0	10677	178	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 (178) 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:292:ALA:HA	4:D:850:HOH:O	1.68	0.94
1:C:91:ARG:HB2	4:C:1389:HOH:O	1.67	0.93
1:D:36:ILE:HD11	1:D:73:LEU:HD23	1.56	0.84
1:B:292:ALA:O	4:B:792:HOH:O	1.95	0.83
1:D:227:TYR:HE1	4:D:926:HOH:O	1.63	0.80
1:C:197:GLN:HE22	1:D:50:MET:HA	1.46	0.80
1:A:350:ASP:HB3	4:A:1440:HOH:O	1.82	0.79
2:C:753:ACO:H141	2:C:753:ACO:H32	1.64	0.79
1:A:173:TRP:O	1:A:176:GLN:HG3	1.83	0.79
1:B:286:HIS:HE1	4:B:775:HOH:O	1.65	0.79
1:A:286:HIS:HE1	4:A:1446:HOH:O	1.66	0.78
2:A:751:ACO:O	4:A:1472:HOH:O	2.00	0.78
1:C:91:ARG:NH1	2:C:753:ACO:O7A	2.18	0.77
1:B:322:ALA:O	1:B:323:ASN:C	2.23	0.76
1:D:68:GLU:O	1:D:72:LYS:HG3	1.88	0.74
1:A:21:HIS:HD2	1:A:161:SER:OG	1.72	0.72
1:D:261:PRO:HA	4:D:791:HOH:O	1.88	0.72
2:A:751:ACO:H141	2:A:751:ACO:O5P	1.89	0.72
4:A:1420:HOH:O	1:B:50:MET:HE3	1.89	0.72
1:B:91:ARG:NH1	2:B:752:ACO:O9A	2.24	0.70
1:D:109:ALA:HB1	1:D:164:LEU:HD11	1.73	0.70
1:C:285:ASP:OD2	4:C:1406:HOH:O	2.09	0.69
1:D:103:ASN:HD22	1:D:103:ASN:C	1.96	0.68
1:A:2:ALA:HB1	4:A:1406:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:754:ACO:H141	2:D:754:ACO:H31	1.75	0.68
1:C:48:ASP:OD1	1:C:50:MET:HB3	1.93	0.68
1:B:21:HIS:HA	1:B:50:MET:HE1	1.77	0.67
1:C:223:TYR:OH	1:C:263:ASN:ND2	2.27	0.67
1:C:148:VAL:HB	4:D:915:HOH:O	1.96	0.66
2:D:754:ACO:S1P	4:D:826:HOH:O	2.54	0.65
1:A:145:GLU:OE2	1:B:145:GLU:OE2	2.15	0.65
1:C:322:ALA:O	1:C:323:ASN:C	2.36	0.64
1:C:76:LYS:HE3	1:C:360:GLY:HA2	1.80	0.64
1:C:130:TYR:HE2	2:C:753:ACO:CH3	2.11	0.63
1:A:349:ILE:HD11	1:A:354:VAL:HG23	1.80	0.63
1:D:237:VAL:HB	4:D:926:HOH:O	1.99	0.62
1:B:322:ALA:O	1:B:323:ASN:O	2.17	0.62
1:C:316:ARG:HD2	1:D:117:THR:O	2.00	0.61
1:C:38:ARG:CZ	1:C:39:PRO:O	2.48	0.61
1:B:85:ARG:HD3	4:B:774:HOH:O	2.01	0.61
1:C:302:LEU:HD12	4:D:917:HOH:O	1.99	0.61
1:D:53:ASN:OD1	1:D:343:ARG:NH1	2.34	0.60
1:B:21:HIS:HD2	1:B:161:SER:OG	1.84	0.60
1:C:130:TYR:HE2	2:C:753:ACO:HH33	1.67	0.58
1:B:130:TYR:CE2	1:B:188:MET:HE3	2.39	0.58
1:D:19:GLY:HA3	4:D:799:HOH:O	2.04	0.58
1:C:185:ASP:HB3	1:D:333:ARG:HB2	1.85	0.57
1:B:259:LEU:HD13	1:B:274:LEU:HD13	1.88	0.56
2:C:753:ACO:HN4	2:C:753:ACO:HH33	1.71	0.55
1:A:36:ILE:HD11	1:A:73:LEU:HD23	1.88	0.55
1:C:5:LEU:HD23	1:D:173:TRP:CD1	2.42	0.55
1:A:19:GLY:HA3	4:A:1405:HOH:O	2.07	0.55
1:A:37:ASP:OD1	1:A:38:ARG:N	2.39	0.54
1:A:259:LEU:HD22	1:A:274:LEU:HD13	1.90	0.54
1:A:58:THR:HG23	4:A:1377:HOH:O	2.07	0.54
1:A:176:GLN:HE21	1:B:176:GLN:NE2	2.06	0.54
1:C:109:ALA:HB1	1:C:164:LEU:HD11	1.89	0.54
1:C:120:ARG:NH2	1:D:310:GLU:OE2	2.31	0.54
1:C:18:PRO:HB3	1:C:156:ASP:O	2.08	0.53
1:C:259:LEU:HD12	1:C:271:LEU:CD1	2.38	0.53
1:D:80:LEU:HD23	1:D:108:TYR:CE1	2.43	0.53
1:C:302:LEU:O	1:D:135:GLY:HA2	2.09	0.53
1:D:103:ASN:HD22	1:D:105:ARG:H	1.56	0.53
1:B:180:LYS:HG3	4:B:862:HOH:O	2.08	0.53
1:D:103:ASN:C	1:D:103:ASN:ND2	2.63	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:ASN:ND2	1:D:105:ARG:H	2.07	0.52
1:C:169:LEU:HB3	1:D:169:LEU:HB3	1.90	0.52
1:B:45:ILE:HG23	1:B:45:ILE:O	2.10	0.51
1:A:210:ASP:N	3:A:1301:GOL:O1	2.32	0.51
1:B:251:GLY:HA3	1:B:291:PHE:CE2	2.45	0.51
1:C:308:HIS:HA	4:C:1367:HOH:O	2.11	0.51
1:B:198:MET:HE2	1:B:199:MET:HE1	1.93	0.51
1:C:214:ALA:O	1:C:265:ARG:NH2	2.36	0.51
1:C:241:GLU:N	1:C:241:GLU:OE1	2.37	0.51
1:A:135:GLY:HA2	1:B:302:LEU:O	2.11	0.50
1:C:197:GLN:NE2	1:D:50:MET:HA	2.20	0.50
1:C:197:GLN:HE22	1:D:50:MET:CA	2.21	0.50
1:C:198:MET:HG2	1:C:202:MET:HE2	1.94	0.50
1:C:134:ASN:HD22	1:C:134:ASN:C	2.14	0.50
1:C:194:VAL:O	1:D:21:HIS:HE1	1.95	0.50
1:C:91:ARG:CB	4:C:1389:HOH:O	2.40	0.50
1:A:173:TRP:CD1	1:B:5:LEU:HD23	2.47	0.49
1:B:16:ILE:HG22	2:B:752:ACO:S1P	2.53	0.49
1:A:286:HIS:HD2	1:D:253:GLY:HA2	1.77	0.49
1:C:21:HIS:HD2	1:C:161:SER:OG	1.95	0.49
1:D:18:PRO:HB2	1:D:111:MET:HG2	1.94	0.49
1:D:322:ALA:HB1	4:D:901:HOH:O	2.11	0.49
1:C:286:HIS:HE1	4:C:1371:HOH:O	1.95	0.49
1:D:203:ARG:NH2	4:D:896:HOH:O	2.47	0.48
1:C:57:VAL:HG12	1:C:349:ILE:O	2.13	0.48
1:D:65:GLN:HG2	1:D:69:LEU:HD12	1.96	0.48
1:D:292:ALA:CA	4:D:850:HOH:O	2.41	0.48
1:C:188:MET:CE	2:C:753:ACO:HH32	2.44	0.48
1:D:85:ARG:NH1	1:D:122:GLN:OE1	2.47	0.48
1:B:286:HIS:CE1	4:B:775:HOH:O	2.51	0.47
1:B:260:PRO:HG2	1:B:271:LEU:HB2	1.95	0.47
4:C:1403:HOH:O	1:D:173:TRP:HZ3	1.97	0.47
1:C:74:ILE:HG12	1:C:80:LEU:HD13	1.95	0.47
1:C:119:PRO:HB2	4:D:888:HOH:O	2.15	0.47
1:C:72:LYS:HA	4:C:1402:HOH:O	2.14	0.47
1:B:352:GLU:HA	1:B:355:LEU:HD12	1.97	0.47
1:A:38:ARG:HG2	1:A:39:PRO:HD2	1.95	0.47
1:A:117:THR:O	1:B:316:ARG:HD2	2.15	0.47
1:B:85:ARG:HB2	2:B:752:ACO:O2A	2.15	0.47
1:A:349:ILE:HD11	1:A:354:VAL:CG2	2.43	0.47
1:C:286:HIS:CE1	4:C:1371:HOH:O	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ILE:HG23	4:D:772:HOH:O	2.14	0.47
1:C:255:ASP:O	1:C:259:LEU:HD23	2.15	0.47
1:D:227:TYR:CE1	4:D:926:HOH:O	2.51	0.46
1:D:251:GLY:HA3	1:D:291:PHE:CE2	2.49	0.46
1:C:317:ASN:N	1:C:317:ASN:HD22	2.14	0.46
1:A:76:LYS:HE2	1:A:358:TRP:O	2.14	0.46
4:C:1399:HOH:O	1:D:204:ALA:HB2	2.15	0.46
1:B:52:ARG:HG3	1:B:342:PRO:HB3	1.97	0.46
1:A:130:TYR:CE2	1:A:188:MET:HE3	2.51	0.46
1:D:69:LEU:HB3	1:D:351:ILE:HD13	1.96	0.46
1:D:145:GLU:O	1:D:212:ARG:NH2	2.47	0.45
1:C:105:ARG:HB3	1:C:175:ARG:HH11	1.81	0.45
1:B:223:TYR:OH	1:B:263:ASN:ND2	2.43	0.45
1:C:117:THR:O	1:D:316:ARG:HD2	2.17	0.45
1:D:89:THR:OG1	1:D:110:ARG:NH2	2.50	0.45
1:C:299:THR:HG23	4:C:1352:HOH:O	2.17	0.45
1:A:131:ILE:HA	1:A:134:ASN:HD21	1.81	0.45
1:A:349:ILE:HD12	1:A:350:ASP:O	2.16	0.45
1:B:252:LEU:HD21	1:B:279:PHE:CE1	2.52	0.45
1:C:145:GLU:O	1:C:212:ARG:NH2	2.44	0.45
4:C:1417:HOH:O	1:D:217:LEU:HB3	2.17	0.45
1:A:198:MET:HB2	4:A:1420:HOH:O	2.16	0.45
1:B:150:PRO:HG2	4:B:753:HOH:O	2.17	0.45
1:D:323:ASN:O	1:D:324:GLY:O	2.35	0.44
1:B:18:PRO:HB3	1:B:156:ASP:O	2.17	0.44
1:B:286:HIS:HD2	4:B:885:HOH:O	1.99	0.44
1:A:50:MET:HA	1:B:197:GLN:HE22	1.83	0.44
1:C:259:LEU:HD13	1:C:274:LEU:HD13	2.00	0.44
1:A:302:LEU:O	1:B:135:GLY:HA2	2.17	0.44
1:C:141:GLY:HA3	4:C:1374:HOH:O	2.17	0.44
1:D:208:TRP:CZ3	1:D:215:ASN:HB3	2.52	0.44
1:D:18:PRO:HB2	1:D:111:MET:CG	2.47	0.44
1:D:203:ARG:HD2	1:D:210:ASP:OD1	2.18	0.44
1:B:13:LEU:HD12	1:B:82:GLU:HB3	2.00	0.44
1:C:157:PHE:O	1:C:162:MET:HG2	2.18	0.44
1:C:135:GLY:HA2	1:D:302:LEU:O	2.18	0.43
1:A:209:THR:HB	3:A:1301:GOL:H12	2.00	0.43
1:D:277:GLU:HG3	4:D:909:HOH:O	2.18	0.43
1:A:21:HIS:CD2	1:A:161:SER:OG	2.62	0.43
1:A:21:HIS:HE1	1:B:194:VAL:O	2.01	0.43
1:A:286:HIS:CE1	4:A:1446:HOH:O	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ALA:HB1	1:C:327:GLN:OE1	2.18	0.43
1:B:263:ASN:ND2	4:B:899:HOH:O	2.50	0.43
1:D:237:VAL:HG22	1:D:298:VAL:HG22	2.00	0.43
1:A:292:ALA:O	1:B:123:GLN:NE2	2.50	0.43
1:D:17:GLY:O	1:D:20:PRO:HD2	2.18	0.43
1:A:113:GLY:HA3	1:A:130:TYR:CZ	2.53	0.43
1:B:80:LEU:HD23	1:B:108:TYR:CE1	2.54	0.42
1:C:130:TYR:HE2	2:C:753:ACO:HH31	1.82	0.42
1:A:89:THR:OG1	1:A:110:ARG:NH2	2.53	0.42
1:B:310:GLU:O	1:B:314:ILE:HG13	2.18	0.42
1:C:242:PRO:HD2	4:C:1343:HOH:O	2.19	0.42
1:D:268:TRP:N	1:D:269:PRO:CD	2.83	0.42
2:C:753:ACO:N4P	2:C:753:ACO:HH33	2.35	0.42
1:C:200:TRP:C	1:D:327:GLN:HE22	2.23	0.42
1:D:25:ILE:O	1:D:29:LEU:HG	2.20	0.41
1:A:345:PRO:HB3	4:A:1463:HOH:O	2.20	0.41
1:A:5:LEU:HD21	1:B:170:ALA:HA	2.02	0.41
1:C:91:ARG:CG	4:C:1389:HOH:O	2.67	0.41
1:D:145:GLU:HG3	1:D:146:ARG:O	2.20	0.41
1:B:134:ASN:HD22	1:B:134:ASN:C	2.23	0.41
1:A:18:PRO:HB3	1:A:156:ASP:O	2.21	0.41
1:A:260:PRO:HG2	1:A:271:LEU:HB2	2.03	0.41
1:C:156:ASP:OD1	2:C:753:ACO:HH32	2.20	0.41
1:C:223:TYR:O	1:C:237:VAL:HG12	2.21	0.41
1:B:156:ASP:HA	1:B:188:MET:SD	2.61	0.40
1:C:144:ASP:OD1	4:C:1419:HOH:O	2.22	0.40
1:D:21:HIS:HD2	1:D:161:SER:OG	2.05	0.40
1:D:343:ARG:HA	1:D:344:PRO:HD2	1.82	0.40
1:B:29:LEU:HA	1:B:339:SER:OG	2.20	0.40
1:D:28:ASP:HB3	1:D:330:PRO:HB3	2.03	0.40
1:C:136:ILE:HG21	1:C:154:VAL:HG11	2.03	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	357/360 (99%)	341 (96%)	15 (4%)	1 (0%)	41	50
1	B	354/360 (98%)	338 (96%)	15 (4%)	1 (0%)	41	50
1	C	351/360 (98%)	335 (95%)	15 (4%)	1 (0%)	41	50
1	D	351/360 (98%)	333 (95%)	16 (5%)	2 (1%)	25	31
All	All	1413/1440 (98%)	1347 (95%)	61 (4%)	5 (0%)	34	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	292	ALA
1	A	292	ALA
1	B	323	ASN
1	D	324	GLY
1	C	323	ASN

### 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	277/275 (101%)	269 (97%)	8 (3%)	42	58
1	B	274/275 (100%)	263 (96%)	11 (4%)	31	44
1	C	271/275 (98%)	261 (96%)	10 (4%)	34	48
1	D	271/275 (98%)	265 (98%)	6 (2%)	52	69
All	All	1093/1100 (99%)	1058 (97%)	35 (3%)	39	54

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ILE
1	A	91	ARG
1	A	134	ASN

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Mol	Chain	Res	Type
1	A	176	GLN
1	A	177	SER
1	A	199	MET
1	A	349	ILE
1	A	359	ASP
1	B	37	ASP
1	B	38	ARG
1	B	50	MET
1	B	58	THR
1	B	76	LYS
1	B	103	ASN
1	B	133	LEU
1	B	134	ASN
1	B	199	MET
1	B	323	ASN
1	B	349	ILE
1	C	38	ARG
1	C	50	MET
1	C	58	THR
1	C	103	ASN
1	C	134	ASN
1	C	199	MET
1	C	293	ASN
1	C	323	ASN
1	C	349	ILE
1	C	359	ASP
1	D	103	ASN
1	D	134	ASN
1	D	199	MET
1	D	259	LEU
1	D	356	THR
1	D	359	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	103	ASN
1	A	123	GLN
1	A	134	ASN
1	A	176	GLN
1	A	286	HIS

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Mol	Chain	Res	Type
1	A	327	GLN
1	B	21	HIS
1	B	103	ASN
1	B	134	ASN
1	B	176	GLN
1	B	263	ASN
1	B	286	HIS
1	C	21	HIS
1	C	65	GLN
1	C	103	ASN
1	C	134	ASN
1	C	263	ASN
1	C	317	ASN
1	D	21	HIS
1	D	65	GLN
1	D	103	ASN
1	D	123	GLN
1	D	134	ASN
1	D	263	ASN
1	D	286	HIS
1	D	327	GLN
1	D	341	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 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
2	ACO	A	751	-	45,53,53	0.88	1 (2%)	56,79,79	1.28	7 (12%)
2	ACO	D	754	-	45,53,53	0.93	2 (4%)	56,79,79	1.28	6 (10%)
3	GOL	A	1301	-	5,5,5	0.78	0	5,5,5	2.09	2 (40%)
2	ACO	C	753	-	45,53,53	0.87	1 (2%)	56,79,79	1.12	5 (8%)
3	GOL	C	1302	-	5,5,5	0.34	0	5,5,5	0.34	0
2	ACO	B	752	-	45,53,53	0.90	3 (6%)	56,79,79	1.20	4 (7%)

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	A	751	-	-	15/47/67/67	0/3/3/3
2	ACO	D	754	-	-	18/47/67/67	0/3/3/3
3	GOL	A	1301	-	-	1/4/4/4	-
2	ACO	C	753	-	-	9/47/67/67	0/3/3/3
3	GOL	C	1302	-	-	4/4/4/4	-
2	ACO	B	752	-	-	12/47/67/67	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	753	ACO	C5A-C4A	2.87	1.48	1.40
2	D	754	ACO	O4B-C1B	2.71	1.44	1.41
2	B	752	ACO	C5A-C4A	2.68	1.48	1.40
2	D	754	ACO	C5A-C4A	2.60	1.47	1.40
2	A	751	ACO	C5A-C4A	2.56	1.47	1.40
2	B	752	ACO	O4B-C1B	2.19	1.44	1.41
2	B	752	ACO	C2A-N3A	2.08	1.35	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	754	ACO	C4A-C5A-N7A	-3.60	105.64	109.40
2	C	753	ACO	N3A-C2A-N1A	-3.55	123.13	128.68
2	A	751	ACO	N3A-C2A-N1A	-3.54	123.14	128.68
2	D	754	ACO	N3A-C2A-N1A	-3.53	123.16	128.68
3	A	1301	GOL	O3-C3-C2	-3.42	93.79	110.20
2	B	752	ACO	N3A-C2A-N1A	-3.40	123.36	128.68
2	A	751	ACO	C4A-C5A-N7A	-3.20	106.06	109.40
3	A	1301	GOL	O1-C1-C2	-3.07	95.50	110.20
2	B	752	ACO	O4B-C1B-C2B	-2.91	102.67	106.93
2	B	752	ACO	C4A-C5A-N7A	-2.86	106.42	109.40
2	A	751	ACO	C6P-C7P-N8P	2.78	117.50	111.90
2	C	753	ACO	C4A-C5A-N7A	-2.69	106.59	109.40
2	C	753	ACO	O4B-C1B-C2B	-2.65	103.06	106.93
2	D	754	ACO	CDP-CBP-CAP	2.63	113.37	108.82
2	D	754	ACO	C2P-S1P-C	2.49	114.76	101.68
2	D	754	ACO	C7P-C6P-C5P	-2.26	108.60	112.36
2	A	751	ACO	P2A-O3A-P1A	-2.26	125.08	132.83
2	C	753	ACO	C2P-S1P-C	2.19	113.22	101.68
2	A	751	ACO	O2A-P1A-O1A	2.17	122.96	112.24
2	A	751	ACO	C7P-N8P-C9P	2.15	126.42	122.59
2	A	751	ACO	CAP-C9P-N8P	2.14	120.83	116.58
2	D	754	ACO	O5P-C5P-C6P	-2.13	118.12	122.02
2	B	752	ACO	C2P-S1P-C	2.11	112.80	101.68
2	C	753	ACO	C2A-N1A-C6A	2.10	122.34	118.75

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	751	ACO	CCP-O6A-P2A-O4A
2	A	751	ACO	CCP-O6A-P2A-O5A
2	A	751	ACO	CAP-C9P-N8P-C7P
2	A	751	ACO	O9P-C9P-N8P-C7P
2	A	751	ACO	C5P-C6P-C7P-N8P
2	A	751	ACO	S1P-C2P-C3P-N4P
2	A	751	ACO	C3P-C2P-S1P-C
2	D	754	ACO	C5B-O5B-P1A-O1A
2	D	754	ACO	CCP-O6A-P2A-O4A
2	D	754	ACO	CCP-O6A-P2A-O5A
2	D	754	ACO	C9P-CAP-CBP-CCP
2	D	754	ACO	C9P-CAP-CBP-CDP
2	D	754	ACO	OAP-CAP-CBP-CEP
2	D	754	ACO	C9P-CAP-CBP-CEP

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Mol	Chain	Res	Type	Atoms
2	D	754	ACO	O-C-S1P-C2P
2	C	753	ACO	C6P-C5P-N4P-C3P
2	C	753	ACO	O5P-C5P-N4P-C3P
2	C	753	ACO	C3P-C2P-S1P-C
2	C	753	ACO	O-C-S1P-C2P
2	C	753	ACO	CH3-C-S1P-C2P
3	C	1302	GOL	O1-C1-C2-C3
2	B	752	ACO	C5B-O5B-P1A-O1A
2	B	752	ACO	CCP-O6A-P2A-O5A
2	B	752	ACO	C6P-C5P-N4P-C3P
2	B	752	ACO	O5P-C5P-N4P-C3P
2	B	752	ACO	C3P-C2P-S1P-C
2	B	752	ACO	O-C-S1P-C2P
2	A	751	ACO	O5P-C5P-N4P-C3P
2	A	751	ACO	C6P-C5P-N4P-C3P
2	A	751	ACO	C6P-C7P-N8P-C9P
2	D	754	ACO	O5P-C5P-N4P-C3P
2	D	754	ACO	C6P-C5P-N4P-C3P
3	C	1302	GOL	O1-C1-C2-O2
2	D	754	ACO	S1P-C2P-C3P-N4P
2	A	751	ACO	O-C-S1P-C2P
2	A	751	ACO	CH3-C-S1P-C2P
2	D	754	ACO	CH3-C-S1P-C2P
2	B	752	ACO	CH3-C-S1P-C2P
2	D	754	ACO	OAP-CAP-CBP-CDP
2	A	751	ACO	CCP-O6A-P2A-O3A
2	D	754	ACO	C5B-O5B-P1A-O3A
2	C	753	ACO	C3B-O3B-P3B-O8A
3	C	1302	GOL	O2-C2-C3-O3
2	B	752	ACO	CCP-O6A-P2A-O3A
2	B	752	ACO	C5B-O5B-P1A-O2A
2	B	752	ACO	CCP-O6A-P2A-O4A
2	D	754	ACO	OAP-CAP-CBP-CCP
3	A	1301	GOL	O1-C1-C2-O2
2	C	753	ACO	P2A-O3A-P1A-O2A
2	D	754	ACO	C3P-C2P-S1P-C
2	A	751	ACO	P1A-O3A-P2A-O6A
2	D	754	ACO	CCP-O6A-P2A-O3A
2	B	752	ACO	C5B-O5B-P1A-O3A
2	A	751	ACO	O4B-C4B-C5B-O5B
2	C	753	ACO	O4B-C4B-C5B-O5B
2	B	752	ACO	O4B-C4B-C5B-O5B

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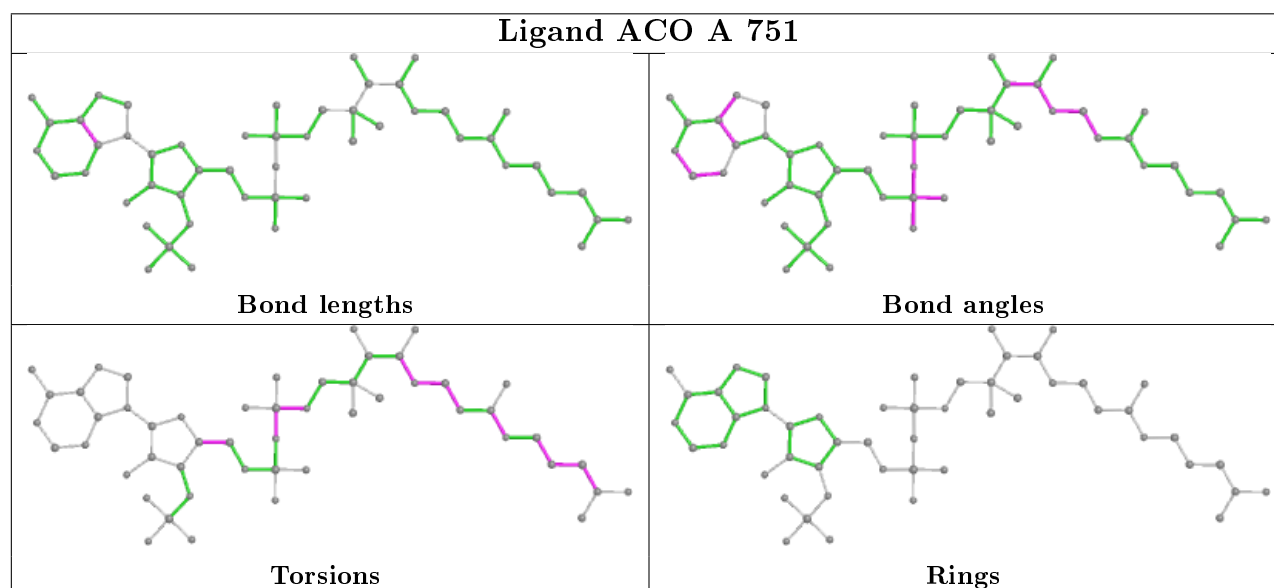
Mol	Chain	Res	Type	Atoms
2	C	753	ACO	P2A-O3A-P1A-O1A
3	C	1302	GOL	C1-C2-C3-O3
2	D	754	ACO	O4B-C4B-C5B-O5B

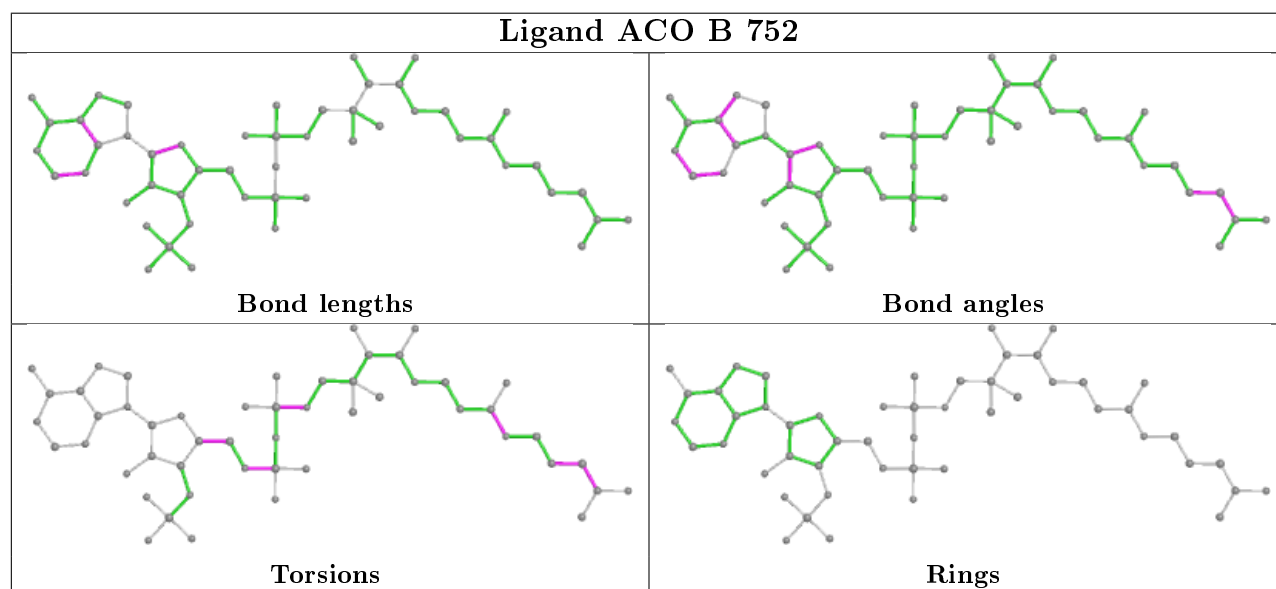
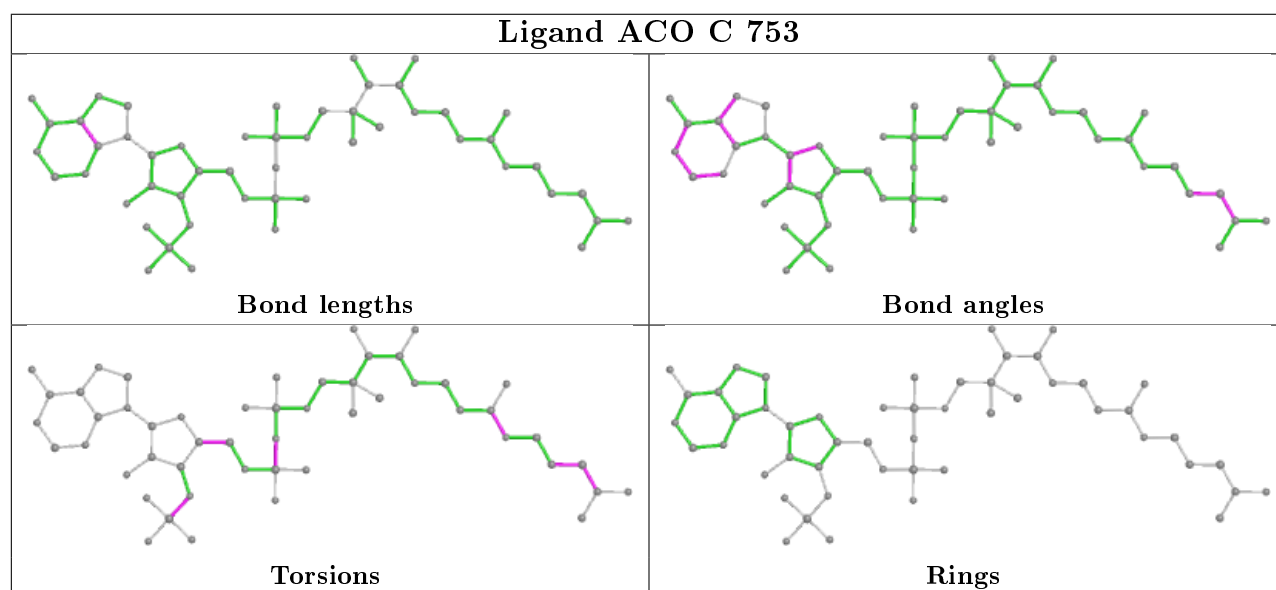
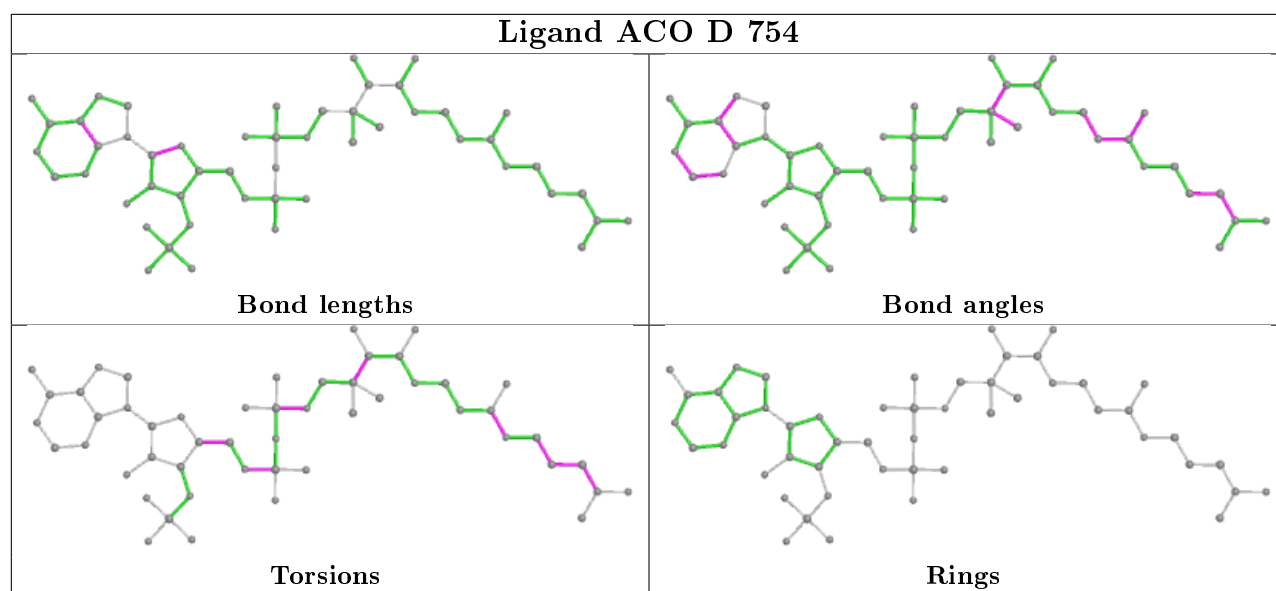
There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	751	ACO	2	0
2	D	754	ACO	2	0
3	A	1301	GOL	2	0
2	C	753	ACO	9	0
2	B	752	ACO	3	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	354/360 (98%)	0.23	5 (1%) 75 80	29, 35, 41, 49	1 (0%)
1	B	354/360 (98%)	0.30	8 (2%) 60 67	30, 35, 41, 47	7 (1%)
1	C	354/360 (98%)	0.31	15 (4%) 36 43	29, 35, 41, 47	12 (3%)
1	D	354/360 (98%)	0.31	11 (3%) 49 56	30, 35, 41, 48	12 (3%)
All	All	1416/1440 (98%)	0.29	39 (2%) 53 60	29, 35, 41, 49	32 (2%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	360	GLY	6.6
1	C	360	GLY	5.6
1	A	360	GLY	5.2
1	B	359	ASP	4.4
1	D	360	GLY	4.4
1	C	359	ASP	4.4
1	B	324	GLY	3.7
1	A	346	ALA	3.6
1	C	322	ALA	3.5
1	C	323	ASN	3.3
1	D	359	ASP	3.3
1	D	322	ALA	3.2
1	C	2	ALA	3.2
1	A	347	ALA	3.1
1	C	349	ILE	3.1
1	B	45	ILE	3.1
1	A	359	ASP	2.9
1	D	349	ILE	2.8
1	B	323	ASN	2.8
1	D	47	ARG	2.7
1	C	347	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	47	ARG	2.5
1	C	346	ALA	2.5
1	D	323	ASN	2.5
1	C	72	LYS	2.4
1	C	345	PRO	2.3
1	C	353	ALA	2.3
1	A	356	THR	2.2
1	D	356	THR	2.2
1	C	356	THR	2.2
1	D	347	ALA	2.2
1	C	357	ASP	2.2
1	C	76	LYS	2.2
1	B	349	ILE	2.1
1	D	45	ILE	2.1
1	D	38	ARG	2.1
1	B	76	LYS	2.1
1	D	324	GLY	2.1
1	B	69	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	GOL	C	1302	6/6	0.76	0.20	58,62,63,64	0
2	ACO	A	751	51/51	0.79	0.23	56,60,76,77	0
2	ACO	B	752	51/51	0.82	0.25	58,62,68,68	0
2	ACO	C	753	51/51	0.85	0.23	51,57,73,74	0
2	ACO	D	754	51/51	0.86	0.17	54,58,66,66	0

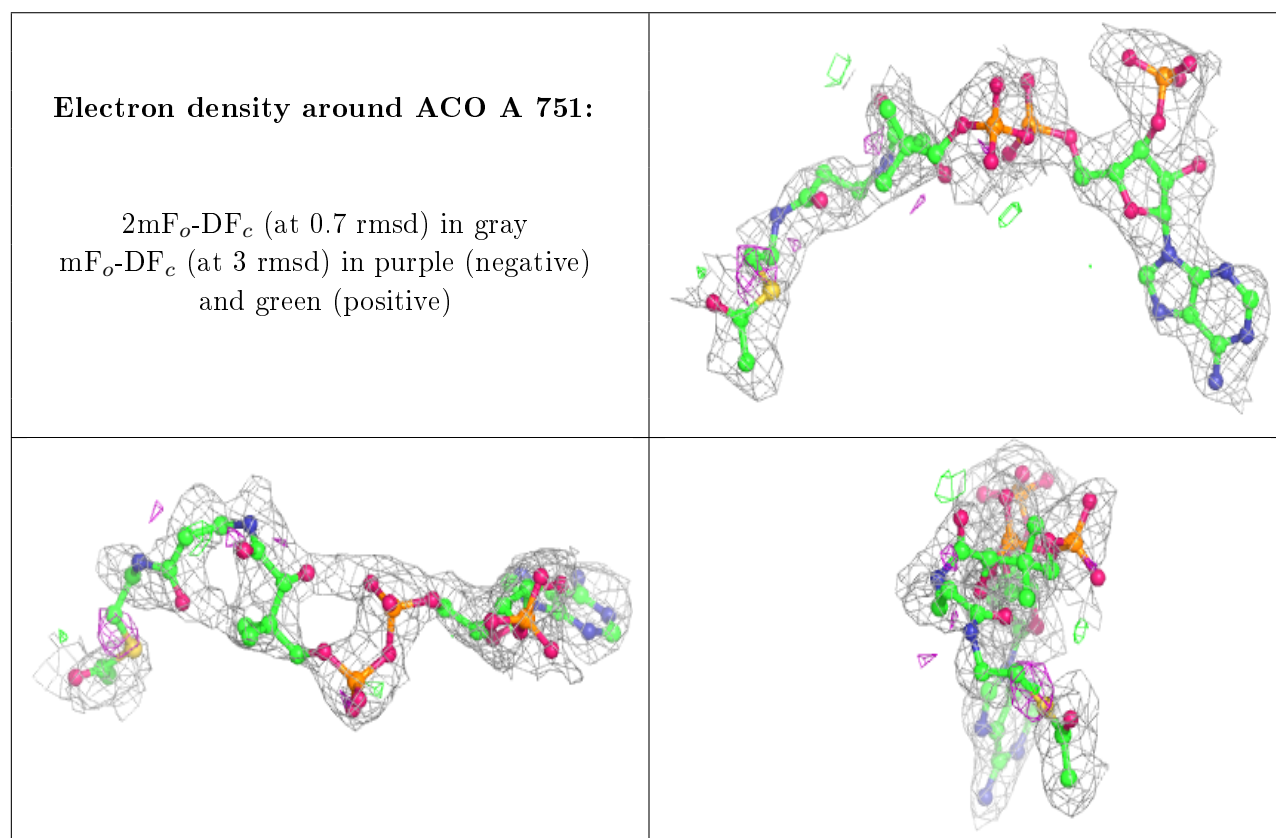
*Continued on next page...*



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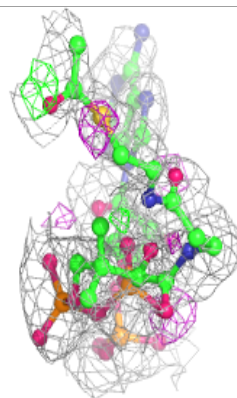
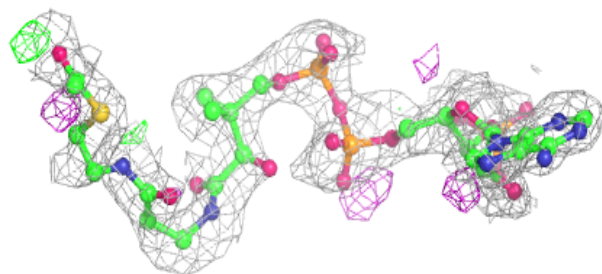
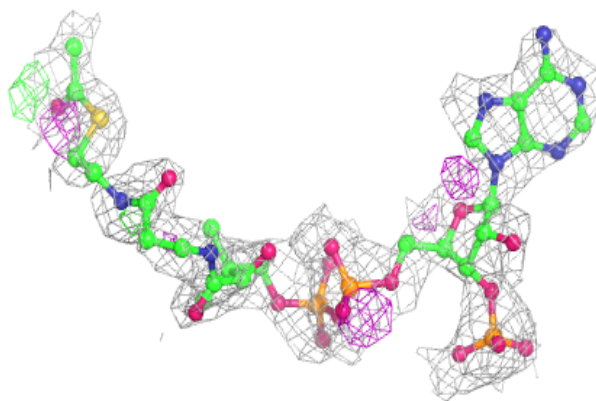
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	1301	6/6	0.94	0.17	21,29,32,32	0

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.

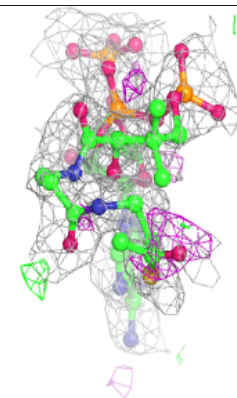
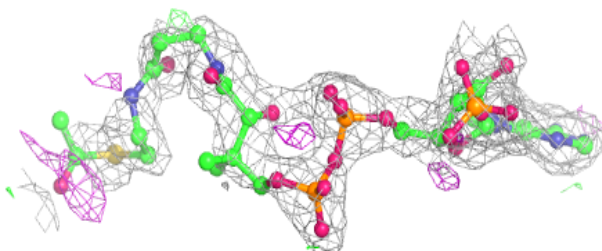
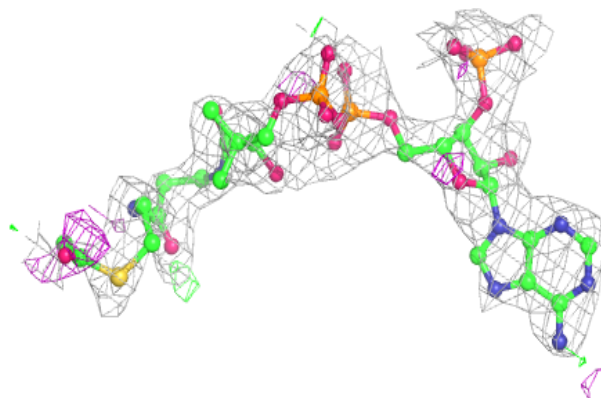


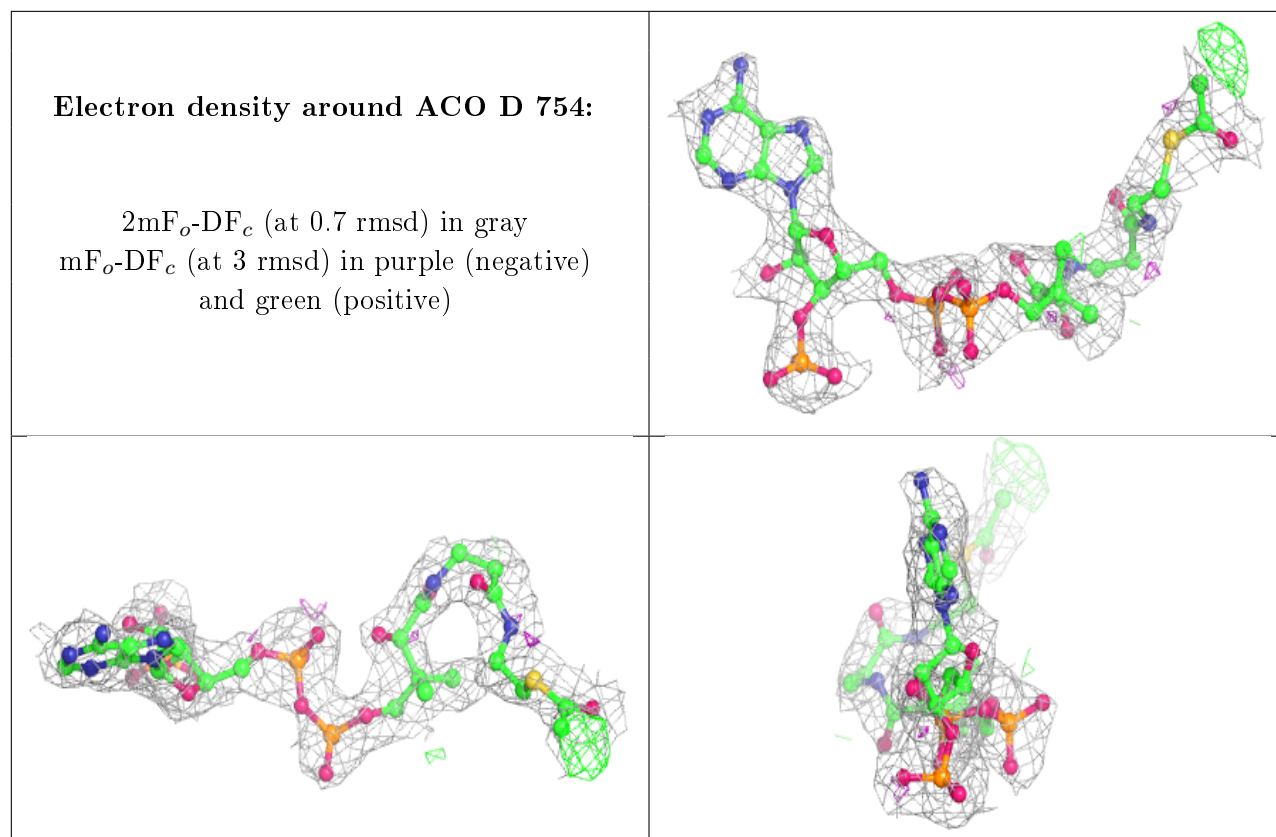
**Electron density around ACO B 752:**

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

**Electron density around ACO C 753:**

$2mF_o-DF_c$  (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.