



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:38 am BST

PDB ID : 4MY0  
Title : Crystal Structure of GCN5-related N-acetyltransferase from *Kribbella flavida*  
Authors : Kim, Y.; Mack, J.; Endres, M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2013-09-26  
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](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

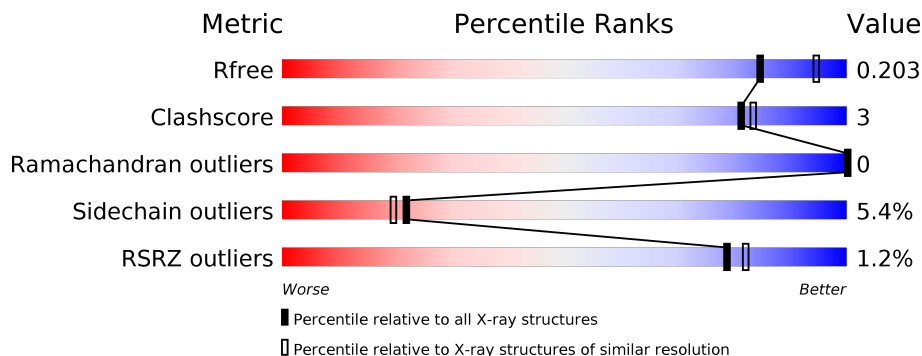
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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 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	392	 2% 90% 8% ..
1	B	392	 2% 91% 8% .
1	C	392	 91% 8% .
1	D	392	 2% 86% 12% ..
1	E	392	 2% 88% 10% ..
1	F	392	 2% 88% 10% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	TRS	A	401	-	X	-	-
3	TRS	C	401	-	X	-	-
3	TRS	D	401	-	X	-	-
3	TRS	E	401	-	X	-	-

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 18874 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 GCN5-related N-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	386	2953	1864	535	549	5	0	1	0
1	B	386	2953	1864	535	549	5	0	1	0
1	C	392	3018	1901	550	562	5	0	3	0
1	D	386	2947	1861	534	547	5	0	0	0
1	E	386	2947	1861	534	547	5	0	0	0
1	F	387	2992	1885	546	556	5	0	4	0

There are 24 discrepancies between the modelled and reference sequences:

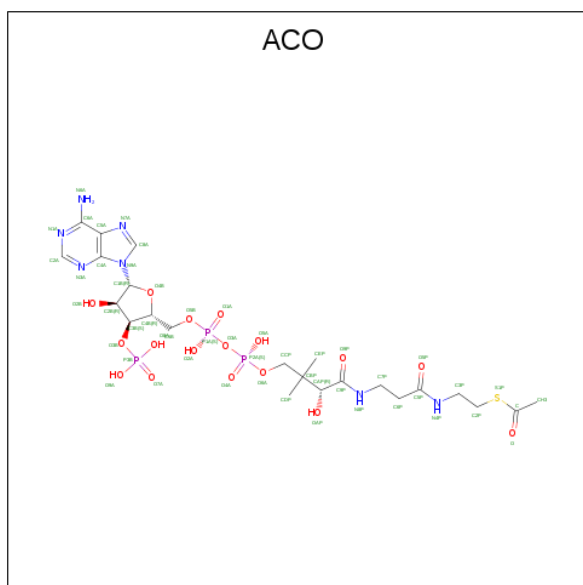
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP D2PVF8
A	-1	ASN	-	EXPRESSION TAG	UNP D2PVF8
A	0	ALA	-	EXPRESSION TAG	UNP D2PVF8
A	1	VAL	MET	SEE REMARK 999	UNP D2PVF8
B	-2	SER	-	EXPRESSION TAG	UNP D2PVF8
B	-1	ASN	-	EXPRESSION TAG	UNP D2PVF8
B	0	ALA	-	EXPRESSION TAG	UNP D2PVF8
B	1	VAL	MET	SEE REMARK 999	UNP D2PVF8
C	-2	SER	-	EXPRESSION TAG	UNP D2PVF8
C	-1	ASN	-	EXPRESSION TAG	UNP D2PVF8
C	0	ALA	-	EXPRESSION TAG	UNP D2PVF8
C	1	VAL	MET	SEE REMARK 999	UNP D2PVF8
D	-2	SER	-	EXPRESSION TAG	UNP D2PVF8
D	-1	ASN	-	EXPRESSION TAG	UNP D2PVF8
D	0	ALA	-	EXPRESSION TAG	UNP D2PVF8
D	1	VAL	MET	SEE REMARK 999	UNP D2PVF8
E	-2	SER	-	EXPRESSION TAG	UNP D2PVF8

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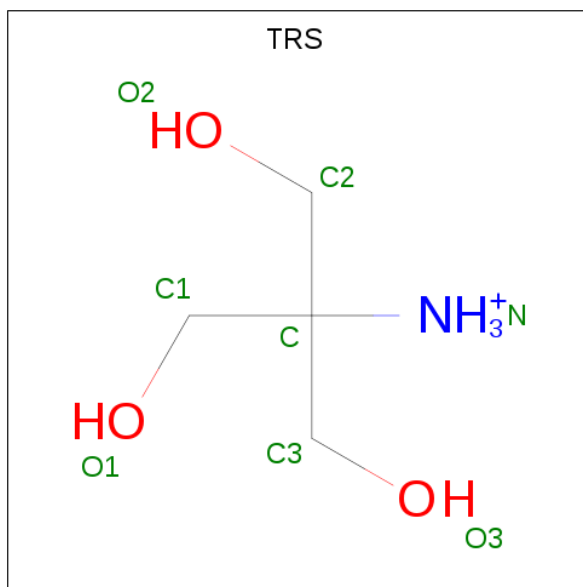
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	EXPRESSION TAG	UNP D2PVF8
E	0	ALA	-	EXPRESSION TAG	UNP D2PVF8
E	1	VAL	MET	SEE REMARK 999	UNP D2PVF8
F	-2	SER	-	EXPRESSION TAG	UNP D2PVF8
F	-1	ASN	-	EXPRESSION TAG	UNP D2PVF8
F	0	ALA	-	EXPRESSION TAG	UNP D2PVF8
F	1	VAL	MET	SEE REMARK 999	UNP D2PVF8

- 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	
			Total	C	N	O	P			S
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



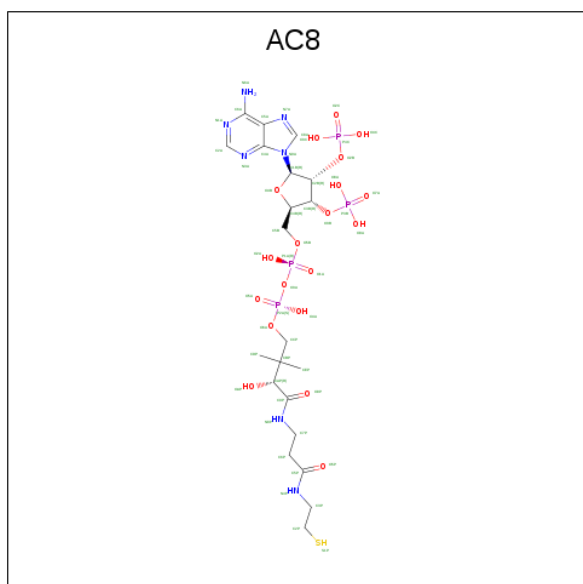
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total 8	C 4	N 1	O 3	0	0
3	B	1	Total 8	C 4	N 1	O 3	0	0
3	C	1	Total 8	C 4	N 1	O 3	0	0
3	D	1	Total 8	C 4	N 1	O 3	0	0
3	E	1	Total 8	C 4	N 1	O 3	0	0
3	F	1	Total 8	C 4	N 1	O 3	0	0

- Molecule 4 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
4	A	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is [(2R,3R,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-bis(phosphonoxy)tetrahydrofuran-2-yl]methyl (3R)-3-hydroxy-2,2-dimethyl-4-oxo-4-({3-oxo-3-[(2-sulfanylethyl)amino]propyl}amino)butyl dihydrogen diphosphate (three-letter code: AC8) (formula: C<sub>21</sub>H<sub>37</sub>N<sub>7</sub>O<sub>19</sub>P<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
5	C	1	52	21	7	19	4	1	0	0

- Molecule 6 is water.

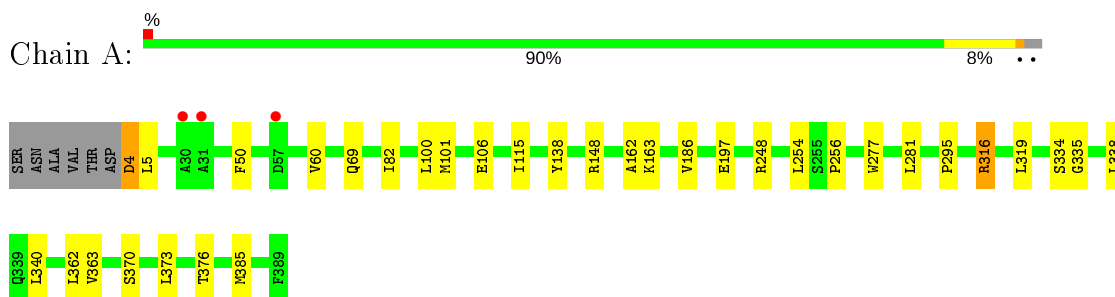
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	156	Total 156	O 156	0	0
6	B	142	Total 142	O 142	0	0
6	C	116	Total 116	O 116	0	0
6	D	77	Total 77	O 77	0	0
6	E	91	Total 91	O 91	0	0
6	F	130	Total 130	O 130	0	0



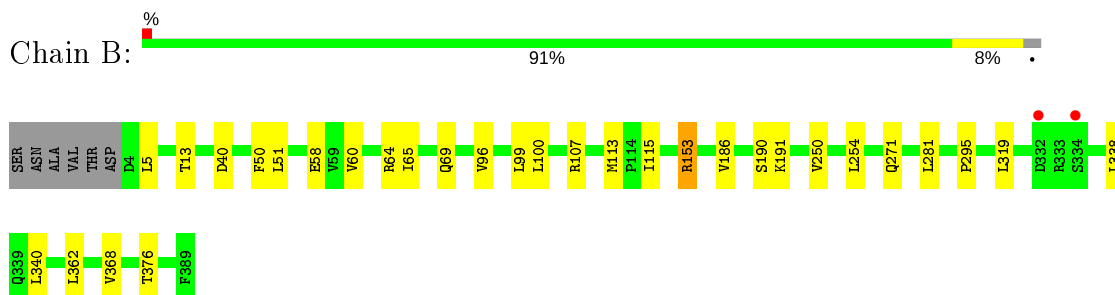
### 3 Residue-property plots [i](#)

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.

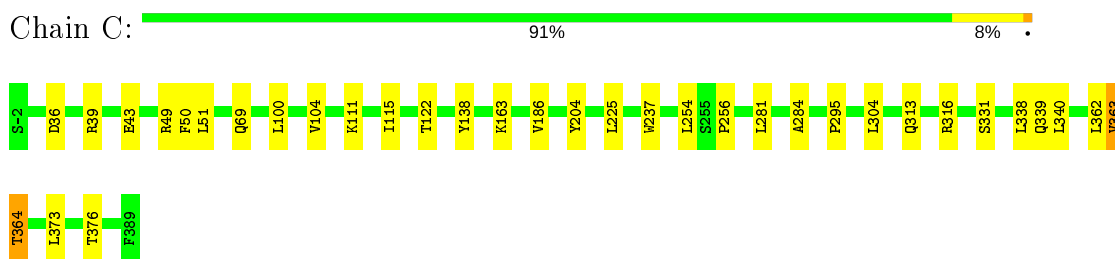
- Molecule 1: GCN5-related N-acetyltransferase



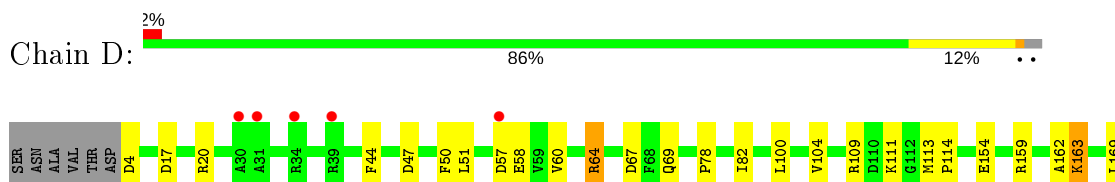
- Molecule 1: GCN5-related N-acetyltransferase



- Molecule 1: GCN5-related N-acetyltransferase

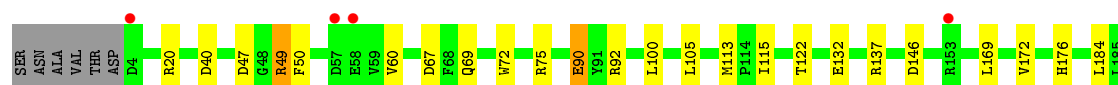
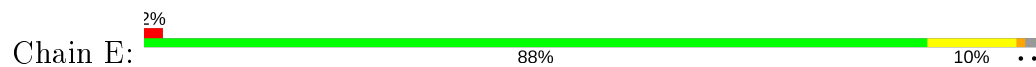


- Molecule 1: GCN5-related N-acetyltransferase

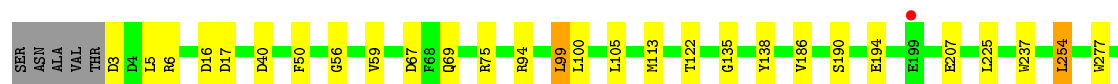
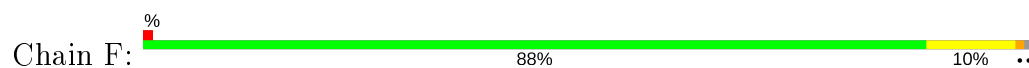




- Molecule 1: GCN5-related N-acetyltransferase



- Molecule 1: GCN5-related N-acetyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.14Å 166.52Å 183.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.91 – 2.10 46.03 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (36.91-2.10) 99.2 (46.03-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1161)	Depositor
R, $R_{free}$	0.166 , 0.202 0.167 , 0.203	Depositor DCC
$R_{free}$ test set	8200 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtrriage
Anisotropy	0.192	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18874	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, TRS, AC8, 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	0.40	0/3016	0.53	0/4095
1	B	0.41	0/3016	0.53	0/4095
1	C	0.39	0/3082	0.53	0/4184
1	D	0.35	0/3010	0.51	0/4086
1	E	0.35	0/3010	0.53	0/4086
1	F	0.39	0/3055	0.55	1/4146 (0.0%)
All	All	0.38	0/18189	0.53	1/24692 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	99	LEU	CA-CB-CG	5.20	127.26	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	2953	0	2879	15	0
1	B	2953	0	2879	10	0
1	C	3018	0	2938	15	0
1	D	2947	0	2874	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2947	0	2874	16	0
1	F	2992	0	2914	21	0
2	A	48	0	31	0	0
2	B	48	0	31	1	0
2	D	48	0	31	0	0
2	E	48	0	31	2	0
2	F	48	0	31	0	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
3	C	8	0	12	0	0
3	D	8	0	12	0	0
3	E	8	0	12	1	0
3	F	8	0	12	0	0
4	A	6	0	8	0	0
4	E	6	0	8	0	0
5	C	52	0	31	1	0
6	A	156	0	0	0	0
6	B	142	0	0	1	0
6	C	116	0	0	0	0
6	D	77	0	0	0	0
6	E	91	0	0	0	0
6	F	130	0	0	0	0
All	All	18874	0	17632	94	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 3.

All (94) 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:F:67:ASP:HA	1:F:113:MSE:HE1	1.63	0.79
1:A:338:LEU:HD11	1:A:363:VAL:HG13	1.71	0.71
1:D:163:LYS:HD2	1:D:163:LYS:H	1.56	0.70
1:A:162:ALA:HB2	1:A:197:GLU:HG3	1.75	0.66
1:E:69:GLN:HB2	1:E:186:VAL:HB	1.76	0.66
1:F:6[B]:ARG:HH12	1:F:56:GLY:H	1.42	0.66
1:A:148:ARG:NH2	5:C:400:AC8:O3C	2.29	0.65
1:D:162:ALA:HB2	1:D:197:GLU:HG3	1.81	0.63
1:E:67:ASP:HA	1:E:113:MSE:HE1	1.81	0.62
1:C:304:LEU:HD23	1:C:339[A]:GLN:HG2	1.83	0.60
1:F:302:ASP:OD2	1:F:316:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:PRO:O	1:B:376:THR:HG21	2.04	0.58
1:B:69:GLN:HB2	1:B:186:VAL:HB	1.86	0.58
1:E:47:ASP:OD2	1:E:49:ARG:NH1	2.37	0.57
1:F:6[B]:ARG:NH2	1:F:56:GLY:O	2.38	0.57
1:A:316:ARG:NH1	1:A:335:GLY:O	2.39	0.56
1:B:115:ILE:HG22	1:B:281:LEU:HD22	1.88	0.56
1:D:69:GLN:HB2	1:D:186:VAL:HB	1.87	0.56
1:F:316:ARG:NH1	1:F:335:GLY:O	2.38	0.56
1:C:36:ASP:OD2	1:C:39:ARG:NH2	2.36	0.56
1:C:69:GLN:HB2	1:C:186:VAL:HB	1.87	0.56
1:D:67:ASP:HA	1:D:113:MSE:HE1	1.88	0.55
1:A:115:ILE:HG22	1:A:281:LEU:HD22	1.87	0.54
1:C:204:TYR:CE1	1:E:90:GLU:HG3	2.43	0.53
1:F:75:ARG:NH2	1:F:289:ALA:O	2.41	0.53
1:D:44:PHE:CD1	1:D:64:ARG:HG2	2.44	0.53
1:F:6[B]:ARG:HH12	1:F:56:GLY:N	2.08	0.52
1:A:376:THR:HG21	1:B:295:PRO:O	2.10	0.52
1:F:17:ASP:HB3	1:F:59:VAL:HB	1.92	0.51
1:D:340:LEU:HB3	1:D:363:VAL:HG22	1.93	0.51
1:B:58:GLU:OE2	1:D:159:ARG:NH2	2.44	0.51
1:E:376:THR:HG21	1:F:295:PRO:O	2.11	0.50
1:E:176:HIS:CE1	1:E:184:LEU:HD13	2.46	0.50
1:E:295:PRO:O	1:F:376:THR:HG21	2.11	0.50
1:D:4:ASP:N	1:D:4:ASP:OD2	2.43	0.50
1:C:295:PRO:O	1:D:376:THR:HG21	2.12	0.49
1:B:64:ARG:NH1	6:B:614:HOH:O	2.44	0.49
1:D:176:HIS:CE1	1:D:184:LEU:HD13	2.47	0.49
1:D:109:ARG:HG2	1:D:282:LEU:HB3	1.95	0.49
1:F:303:LEU:HD22	1:F:340:LEU:HD11	1.94	0.49
1:A:69:GLN:HB2	1:A:186:VAL:HB	1.94	0.49
2:E:400:ACO:S1P	3:E:401:TRS:O2	2.66	0.48
1:F:69:GLN:HB2	1:F:186:VAL:HB	1.93	0.48
1:C:338:LEU:HD11	1:C:363:VAL:HG13	1.96	0.48
1:E:137:ARG:HD3	1:E:275:GLN:OE1	2.13	0.47
1:F:225:LEU:HD13	1:F:237:TRP:CE2	2.50	0.47
1:F:6[B]:ARG:NH1	1:F:56:GLY:H	2.09	0.47
1:B:65:ILE:HG21	1:B:113:MSE:HE1	1.96	0.47
1:C:316:ARG:HG2	1:C:331:SER:HB3	1.96	0.47
1:E:67:ASP:HA	1:E:113:MSE:CE	2.45	0.47
1:A:370:SER:HA	1:A:373:LEU:HD12	1.96	0.47
1:E:132:GLU:HB2	1:E:343:ARG:HB3	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:TRP:CE2	1:A:385:MSE:HE3	2.51	0.46
1:E:115:ILE:HG22	1:E:281:LEU:HD22	1.98	0.45
1:E:75:ARG:NH2	1:E:289:ALA:O	2.47	0.45
1:B:51:LEU:HD11	1:B:107:ARG:HG2	1.98	0.45
1:C:284:ALA:N	1:C:313:GLN:OE1	2.49	0.45
1:A:82:ILE:HD13	1:A:101:MSE:HE1	1.98	0.45
1:F:3:ASP:HB3	1:F:5:LEU:H	1.81	0.45
1:C:376:THR:HG21	1:D:295:PRO:O	2.16	0.45
1:B:153:ARG:HG2	1:B:153:ARG:H	1.52	0.45
1:D:78:PRO:O	1:D:114:PRO:HD2	2.16	0.45
1:F:105:LEU:HD22	1:F:282:LEU:HD21	1.98	0.45
1:F:135:GLY:HA3	1:F:277:TRP:CZ2	2.52	0.45
1:D:277:TRP:CD2	1:D:385:MSE:HE3	2.52	0.45
1:D:307:ASP:OD1	1:D:313:GLN:NE2	2.50	0.44
1:D:17:ASP:OD1	1:D:20:ARG:NH2	2.51	0.44
1:F:301:VAL:HG21	1:F:374:LEU:HD21	2.00	0.44
1:E:146:ASP:CG	1:E:264:VAL:HG22	2.39	0.43
1:A:82:ILE:CD1	1:A:101:MSE:HE1	2.48	0.43
1:C:138:TYR:CD2	1:C:256:PRO:HD3	2.52	0.43
1:E:172:VAL:HG13	1:E:176:HIS:CD2	2.53	0.43
1:A:338:LEU:HD11	1:A:363:VAL:CG1	2.46	0.43
1:C:49:ARG:HG3	1:C:111:LYS:HE3	2.00	0.43
1:C:339[A]:GLN:HB2	1:C:364:THR:HG22	2.00	0.43
1:D:113:MSE:HA	1:D:114:PRO:HD3	1.81	0.43
1:D:47:ASP:O	1:D:111:LYS:NZ	2.32	0.43
1:C:225:LEU:HD13	1:C:237:TRP:CE2	2.54	0.43
1:C:115:ILE:HG22	1:C:281:LEU:HD22	2.01	0.43
1:D:82:ILE:HD12	1:D:104:VAL:HG11	2.00	0.43
1:E:72:TRP:HB3	1:E:291:ARG:HG3	2.01	0.43
1:F:277:TRP:CE2	1:F:385:MSE:HE3	2.55	0.42
1:B:5:LEU:HD13	1:B:96:VAL:HG22	2.00	0.42
1:D:169:LEU:HD23	1:D:169:LEU:HA	1.91	0.41
1:D:191:LYS:HA	1:D:191:LYS:HD3	1.92	0.41
1:A:138:TYR:CD2	1:A:256:PRO:HD3	2.56	0.41
1:F:138:TYR:HB2	1:F:254:LEU:O	2.20	0.41
1:A:4:ASP:OD1	1:A:4:ASP:N	2.54	0.41
1:F:190:SER:O	1:F:194:GLU:HG3	2.21	0.41
1:D:225:LEU:HD13	1:D:237:TRP:CE2	2.56	0.41
1:E:92:ARG:HG2	2:E:400:ACO:OAP	2.20	0.41
2:B:400:ACO:N4P	2:B:400:ACO:H131	2.36	0.41
1:D:318:HIS:HB2	1:D:331:SER:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:LEU:HD12	1:C:104:VAL:HA	2.04	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	385/392 (98%)	384 (100%)	1 (0%)	0	100	100
1	B	385/392 (98%)	383 (100%)	2 (0%)	0	100	100
1	C	393/392 (100%)	391 (100%)	2 (0%)	0	100	100
1	D	384/392 (98%)	383 (100%)	1 (0%)	0	100	100
1	E	384/392 (98%)	383 (100%)	1 (0%)	0	100	100
1	F	389/392 (99%)	388 (100%)	1 (0%)	0	100	100
All	All	2320/2352 (99%)	2312 (100%)	8 (0%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	289/288 (100%)	275 (95%)	14 (5%)	25	24
1	B	289/288 (100%)	272 (94%)	17 (6%)	19	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	296/288 (103%)	285 (96%)	11 (4%)	34	35
1	D	288/288 (100%)	272 (94%)	16 (6%)	21	18
1	E	288/288 (100%)	267 (93%)	21 (7%)	14	11
1	F	293/288 (102%)	279 (95%)	14 (5%)	25	24
All	All	1743/1728 (101%)	1650 (95%)	93 (5%)	22	20

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	5	LEU
1	A	50	PHE
1	A	60	VAL
1	A	100	LEU
1	A	106	GLU
1	A	163	LYS
1	A	248	ARG
1	A	254	LEU
1	A	316	ARG
1	A	319	LEU
1	A	334	SER
1	A	340	LEU
1	A	362	LEU
1	B	13	THR
1	B	40	ASP
1	B	50	PHE
1	B	60	VAL
1	B	99	LEU
1	B	100	LEU
1	B	153	ARG
1	B	190	SER
1	B	191	LYS
1	B	250	VAL
1	B	254	LEU
1	B	271	GLN
1	B	319	LEU
1	B	338	LEU
1	B	340	LEU
1	B	362	LEU
1	B	368	VAL
1	C	43	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	50	PHE
1	C	100	LEU
1	C	122	THR
1	C	163	LYS
1	C	254	LEU
1	C	340	LEU
1	C	362	LEU
1	C	363	VAL
1	C	364	THR
1	C	373	LEU
1	D	50	PHE
1	D	51	LEU
1	D	57	ASP
1	D	58	GLU
1	D	60	VAL
1	D	64	ARG
1	D	100	LEU
1	D	154	GLU
1	D	163	LYS
1	D	217	ASP
1	D	220	LEU
1	D	254	LEU
1	D	332	ASP
1	D	333	ARG
1	D	340	LEU
1	D	373	LEU
1	E	20	ARG
1	E	40	ASP
1	E	49	ARG
1	E	50	PHE
1	E	60	VAL
1	E	90	GLU
1	E	100	LEU
1	E	105	LEU
1	E	122	THR
1	E	169	LEU
1	E	220	LEU
1	E	254	LEU
1	E	255	SER
1	E	264	VAL
1	E	319	LEU
1	E	325	THR

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Mol	Chain	Res	Type
1	E	336	ASP
1	E	340	LEU
1	E	343	ARG
1	E	368	VAL
1	E	373	LEU
1	F	16	ASP
1	F	40	ASP
1	F	50	PHE
1	F	94	ARG
1	F	99	LEU
1	F	100	LEU
1	F	122	THR
1	F	207	GLU
1	F	254	LEU
1	F	333	ARG
1	F	340	LEU
1	F	362	LEU
1	F	363	VAL
1	F	373	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	HIS
1	A	271	GLN
1	A	273	HIS
1	B	271	GLN
1	B	339	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

14 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	B	400	-	41,50,53	0.88	1 (2%)	52,75,79	1.52	9 (17%)
2	ACO	F	400	-	41,50,53	0.82	2 (4%)	52,75,79	1.21	3 (5%)
3	TRS	C	401	-	7,7,7	0.41	0	9,9,9	4.23	5 (55%)
4	GOL	A	402	-	5,5,5	0.31	0	5,5,5	0.51	0
2	ACO	D	400	-	41,50,53	0.81	1 (2%)	52,75,79	1.11	2 (3%)
5	AC8	C	400	-	44,54,54	0.80	2 (4%)	58,82,82	1.37	6 (10%)
3	TRS	E	401	-	7,7,7	0.37	0	9,9,9	4.40	5 (55%)
3	TRS	F	401	-	7,7,7	0.32	0	9,9,9	0.71	0
3	TRS	D	401	-	7,7,7	0.35	0	9,9,9	4.53	6 (66%)
3	TRS	A	401	-	7,7,7	0.41	0	9,9,9	4.24	6 (66%)
3	TRS	B	401	-	7,7,7	0.30	0	9,9,9	0.42	0
2	ACO	A	400	-	41,50,53	0.92	2 (4%)	52,75,79	1.17	2 (3%)
2	ACO	E	400	-	41,50,53	0.87	2 (4%)	52,75,79	1.16	5 (9%)
4	GOL	E	402	-	5,5,5	0.38	0	5,5,5	0.31	0

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	B	400	-	-	16/44/64/67	0/3/3/3
2	ACO	F	400	-	-	5/44/64/67	0/3/3/3
3	TRS	C	401	-	-	5/9/9/9	-
4	GOL	A	402	-	-	1/4/4/4	-
2	ACO	D	400	-	-	4/44/64/67	0/3/3/3
5	AC8	C	400	-	-	3/49/69/69	0/3/3/3
3	TRS	E	401	-	-	7/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRS	F	401	-	-	0/9/9/9	-
3	TRS	D	401	-	-	6/9/9/9	-
3	TRS	A	401	-	-	6/9/9/9	-
3	TRS	B	401	-	-	0/9/9/9	-
2	ACO	A	400	-	-	7/44/64/67	0/3/3/3
2	ACO	E	400	-	-	8/44/64/67	0/3/3/3
4	GOL	E	402	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	ACO	C5A-C4A	2.62	1.47	1.40
2	E	400	ACO	C5A-C4A	2.59	1.47	1.40
2	B	400	ACO	C5A-C4A	2.48	1.47	1.40
2	D	400	ACO	C5A-C4A	2.48	1.47	1.40
2	A	400	ACO	O4B-C1B	2.38	1.44	1.41
2	F	400	ACO	C5A-C4A	2.26	1.46	1.40
5	C	400	AC8	P4C-O2B	2.23	1.63	1.59
2	E	400	ACO	C2A-N3A	2.11	1.35	1.32
2	F	400	ACO	O4B-C1B	2.09	1.44	1.41
5	C	400	AC8	O4B-C1B	2.05	1.43	1.41

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	TRS	C2-C-N	-8.05	83.96	107.98
3	D	401	TRS	C3-C-N	-7.94	84.28	107.98
3	C	401	TRS	C3-C-N	-7.46	85.71	107.98
3	D	401	TRS	C2-C-N	-7.25	86.34	107.98
3	A	401	TRS	C3-C-N	-7.04	86.96	107.98
3	E	401	TRS	C3-C-N	-6.90	87.39	107.98
3	A	401	TRS	C2-C-N	-6.49	88.61	107.98
3	A	401	TRS	C1-C-N	-6.48	88.65	107.98
3	D	401	TRS	C1-C-N	-6.38	88.94	107.98
3	C	401	TRS	C1-C-N	-6.29	89.21	107.98
3	C	401	TRS	C2-C-N	-6.10	89.75	107.98
3	E	401	TRS	C1-C-N	-5.70	90.95	107.98
5	C	400	AC8	N3A-C2A-N1A	-5.28	120.43	128.68
2	B	400	ACO	CEP-CBP-CCP	5.01	116.41	108.23
2	F	400	ACO	N3A-C2A-N1A	-3.75	122.81	128.68
3	E	401	TRS	C3-C-C2	3.63	122.06	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	TRS	C3-C-C1	3.59	121.93	110.81
2	A	400	ACO	N3A-C2A-N1A	-3.48	123.24	128.68
3	C	401	TRS	C3-C-C2	3.46	121.53	110.81
5	C	400	AC8	C3P-N4P-C5P	3.44	129.22	122.84
2	B	400	ACO	N3A-C2A-N1A	-3.42	123.33	128.68
2	E	400	ACO	N3A-C2A-N1A	-3.41	123.35	128.68
2	D	400	ACO	N3A-C2A-N1A	-3.36	123.42	128.68
2	B	400	ACO	CDP-CBP-CAP	3.36	114.65	108.82
3	A	401	TRS	C2-C-C1	3.27	120.96	110.81
3	E	401	TRS	C2-C-C1	3.18	120.67	110.81
5	C	400	AC8	C7P-N8P-C9P	3.10	128.12	122.59
3	D	401	TRS	C2-C-C1	3.05	120.27	110.81
3	D	401	TRS	C3-C-C1	3.00	120.10	110.81
3	A	401	TRS	C3-C-C2	2.90	119.80	110.81
2	A	400	ACO	C4A-C5A-N7A	-2.83	106.45	109.40
2	B	400	ACO	C4A-C5A-N7A	-2.78	106.50	109.40
2	B	400	ACO	C7P-C6P-C5P	-2.76	107.77	112.36
2	F	400	ACO	C4A-C5A-N7A	-2.68	106.61	109.40
2	E	400	ACO	C4A-C5A-N7A	-2.62	106.67	109.40
3	A	401	TRS	C3-C-C1	2.61	118.91	110.81
2	D	400	ACO	C4A-C5A-N7A	-2.60	106.69	109.40
2	F	400	ACO	P2A-O3A-P1A	-2.56	124.03	132.83
3	D	401	TRS	C3-C-C2	2.49	118.55	110.81
2	B	400	ACO	CDP-CBP-CCP	-2.46	104.23	108.23
2	B	400	ACO	O2A-P1A-O1A	2.29	123.57	112.24
5	C	400	AC8	C2P-C3P-N4P	2.29	117.53	112.31
2	E	400	ACO	P2A-O3A-P1A	-2.24	125.15	132.83
5	C	400	AC8	C6P-C7P-N8P	-2.22	107.41	111.90
2	E	400	ACO	C2A-N1A-C6A	2.14	122.42	118.75
2	E	400	ACO	O2A-P1A-O1A	2.14	122.80	112.24
5	C	400	AC8	C7P-C6P-C5P	2.13	115.90	112.36
2	B	400	ACO	O9A-P3B-O8A	2.11	115.72	107.64
2	B	400	ACO	C2A-N1A-C6A	2.11	122.37	118.75

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	400	ACO	C5B-O5B-P1A-O1A
2	B	400	ACO	CCP-O6A-P2A-O3A
2	B	400	ACO	CCP-O6A-P2A-O5A
2	B	400	ACO	CAP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
2	B	400	ACO	OAP-CAP-CBP-CCP
2	B	400	ACO	C9P-CAP-CBP-CCP
2	B	400	ACO	C9P-CAP-CBP-CDP
2	B	400	ACO	OAP-CAP-CBP-CEP
2	B	400	ACO	C9P-CAP-CBP-CEP
3	C	401	TRS	C3-C-C1-O1
3	C	401	TRS	N-C-C1-O1
3	C	401	TRS	C3-C-C2-O2
2	D	400	ACO	C5B-O5B-P1A-O1A
5	C	400	AC8	N8P-C9P-CAP-OAP
5	C	400	AC8	O9P-C9P-CAP-OAP
3	E	401	TRS	C3-C-C1-O1
3	E	401	TRS	N-C-C2-O2
3	D	401	TRS	C3-C-C1-O1
3	D	401	TRS	C3-C-C2-O2
3	D	401	TRS	N-C-C3-O3
3	A	401	TRS	C3-C-C1-O1
3	A	401	TRS	N-C-C1-O1
3	A	401	TRS	C3-C-C2-O2
3	A	401	TRS	N-C-C2-O2
2	A	400	ACO	C5B-O5B-P1A-O1A
2	A	400	ACO	O9P-C9P-CAP-OAP
2	A	400	ACO	N8P-C9P-CAP-OAP
2	E	400	ACO	C5B-O5B-P1A-O1A
4	E	402	GOL	C1-C2-C3-O3
2	B	400	ACO	O5P-C5P-N4P-C3P
2	B	400	ACO	C6P-C5P-N4P-C3P
2	E	400	ACO	C6P-C5P-N4P-C3P
2	A	400	ACO	C6P-C5P-N4P-C3P
5	C	400	AC8	C6P-C7P-N8P-C9P
2	E	400	ACO	O5P-C5P-N4P-C3P
2	A	400	ACO	O5P-C5P-N4P-C3P
2	B	400	ACO	CDP-CBP-CCP-O6A
2	B	400	ACO	CEP-CBP-CCP-O6A
2	F	400	ACO	C6P-C5P-N4P-C3P
2	A	400	ACO	C6P-C7P-N8P-C9P
4	E	402	GOL	O2-C2-C3-O3
2	D	400	ACO	C6P-C7P-N8P-C9P
2	F	400	ACO	O5P-C5P-N4P-C3P
2	D	400	ACO	O5P-C5P-N4P-C3P
2	F	400	ACO	C6P-C7P-N8P-C9P
3	E	401	TRS	C3-C-C2-O2

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Mol	Chain	Res	Type	Atoms
3	E	401	TRS	C2-C-C3-O3
3	D	401	TRS	C2-C-C1-O1
3	D	401	TRS	C2-C-C3-O3
2	D	400	ACO	C6P-C5P-N4P-C3P
2	F	400	ACO	O9P-C9P-CAP-OAP
2	E	400	ACO	O9P-C9P-CAP-OAP
2	B	400	ACO	OAP-CAP-CBP-CDP
2	F	400	ACO	N8P-C9P-CAP-OAP
2	E	400	ACO	N8P-C9P-CAP-OAP
2	B	400	ACO	C5B-O5B-P1A-O3A
2	E	400	ACO	C3B-O3B-P3B-O8A
3	C	401	TRS	C1-C-C3-O3
3	D	401	TRS	N-C-C2-O2
3	A	401	TRS	C1-C-C3-O3
2	E	400	ACO	C6P-C7P-N8P-C9P
3	C	401	TRS	C2-C-C3-O3
3	E	401	TRS	C2-C-C1-O1
3	E	401	TRS	C1-C-C3-O3
3	A	401	TRS	C2-C-C3-O3
4	A	402	GOL	O1-C1-C2-O2
2	A	400	ACO	C5B-O5B-P1A-O3A
2	E	400	ACO	C5B-O5B-P1A-O3A
3	E	401	TRS	C1-C-C2-O2
2	B	400	ACO	C5B-O5B-P1A-O2A

There are no ring outliers.

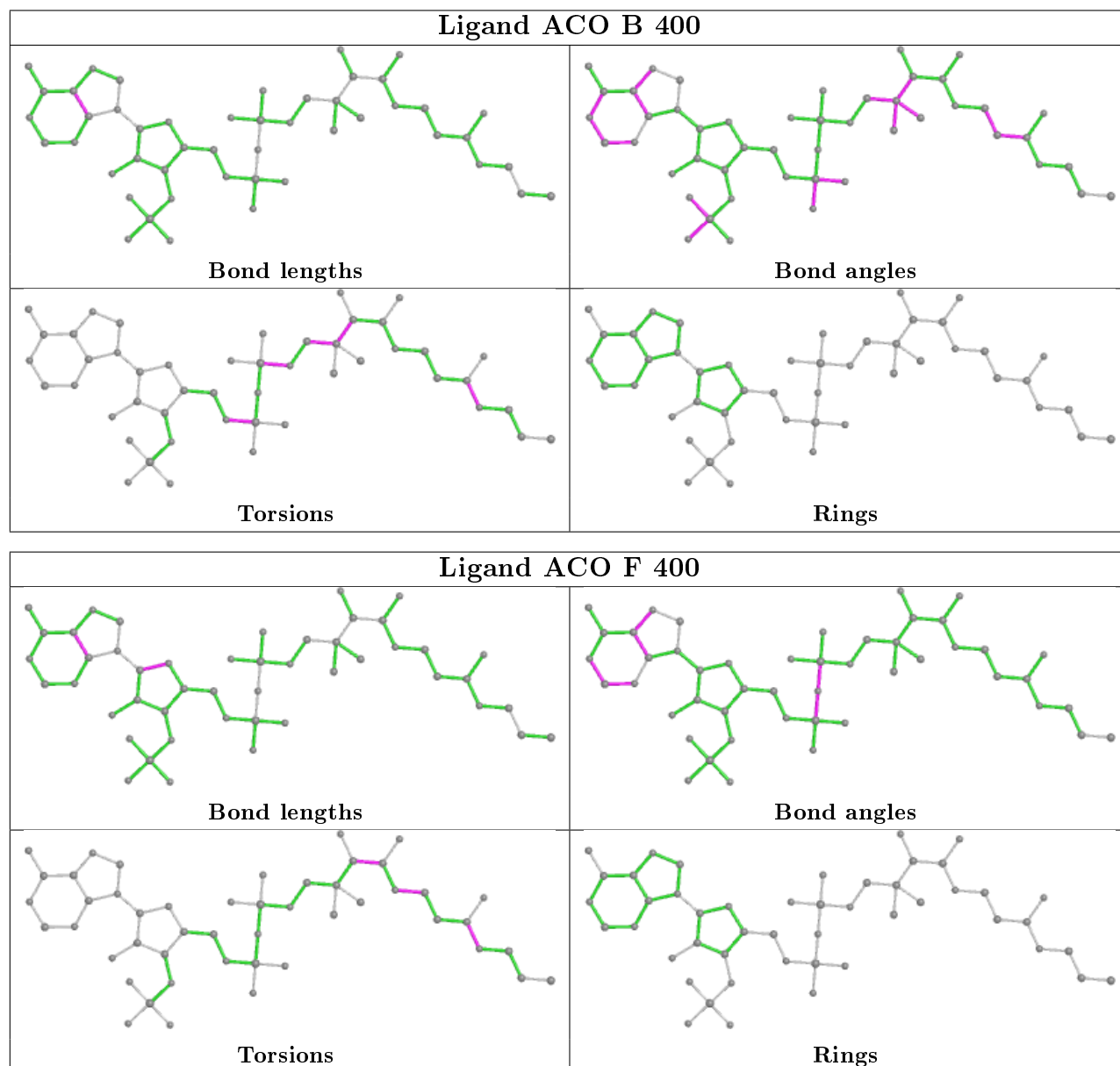
4 monomers are involved in 4 short contacts:

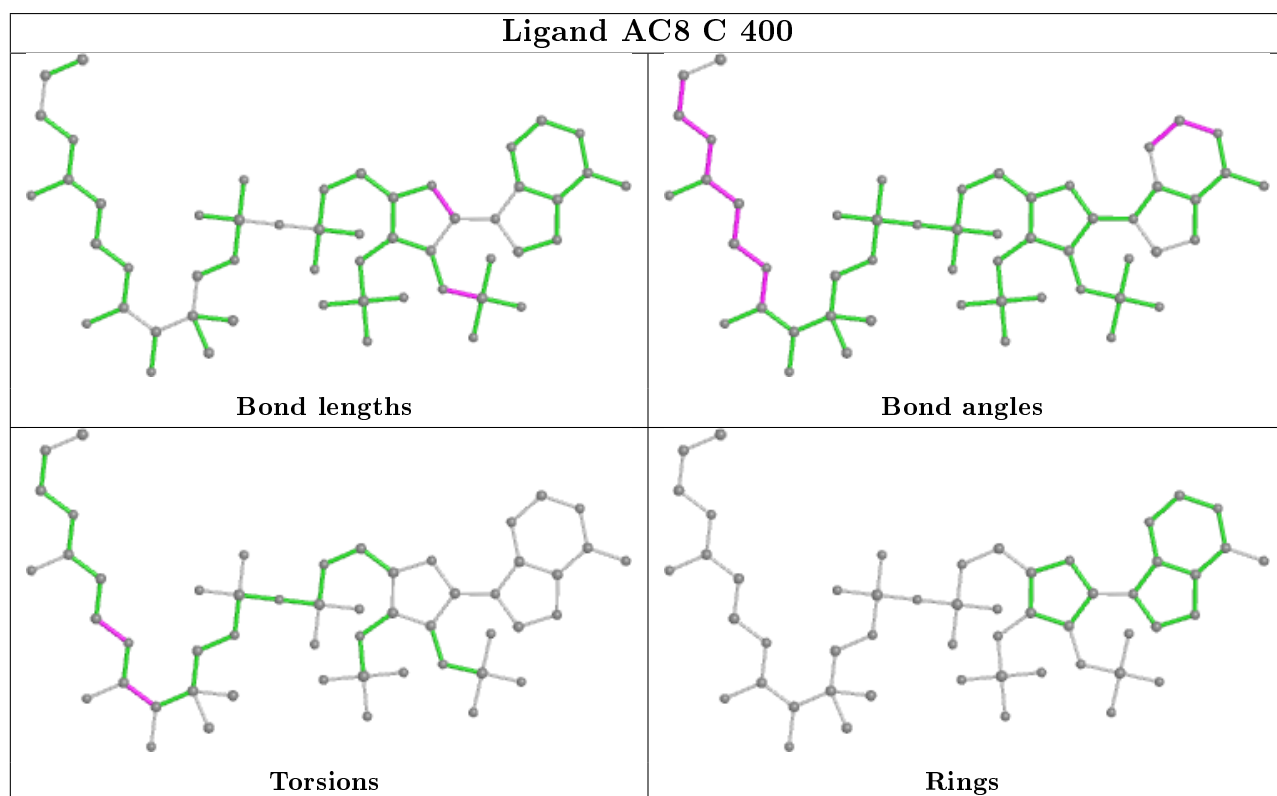
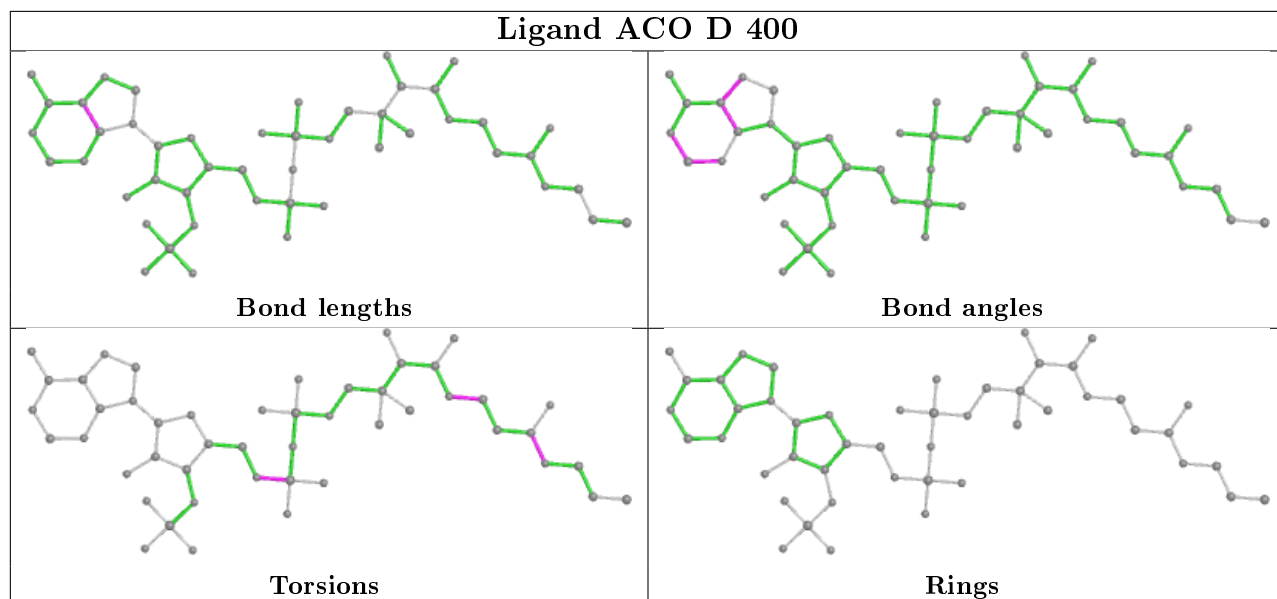
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	ACO	1	0
5	C	400	AC8	1	0
3	E	401	TRS	1	0
2	E	400	ACO	2	0

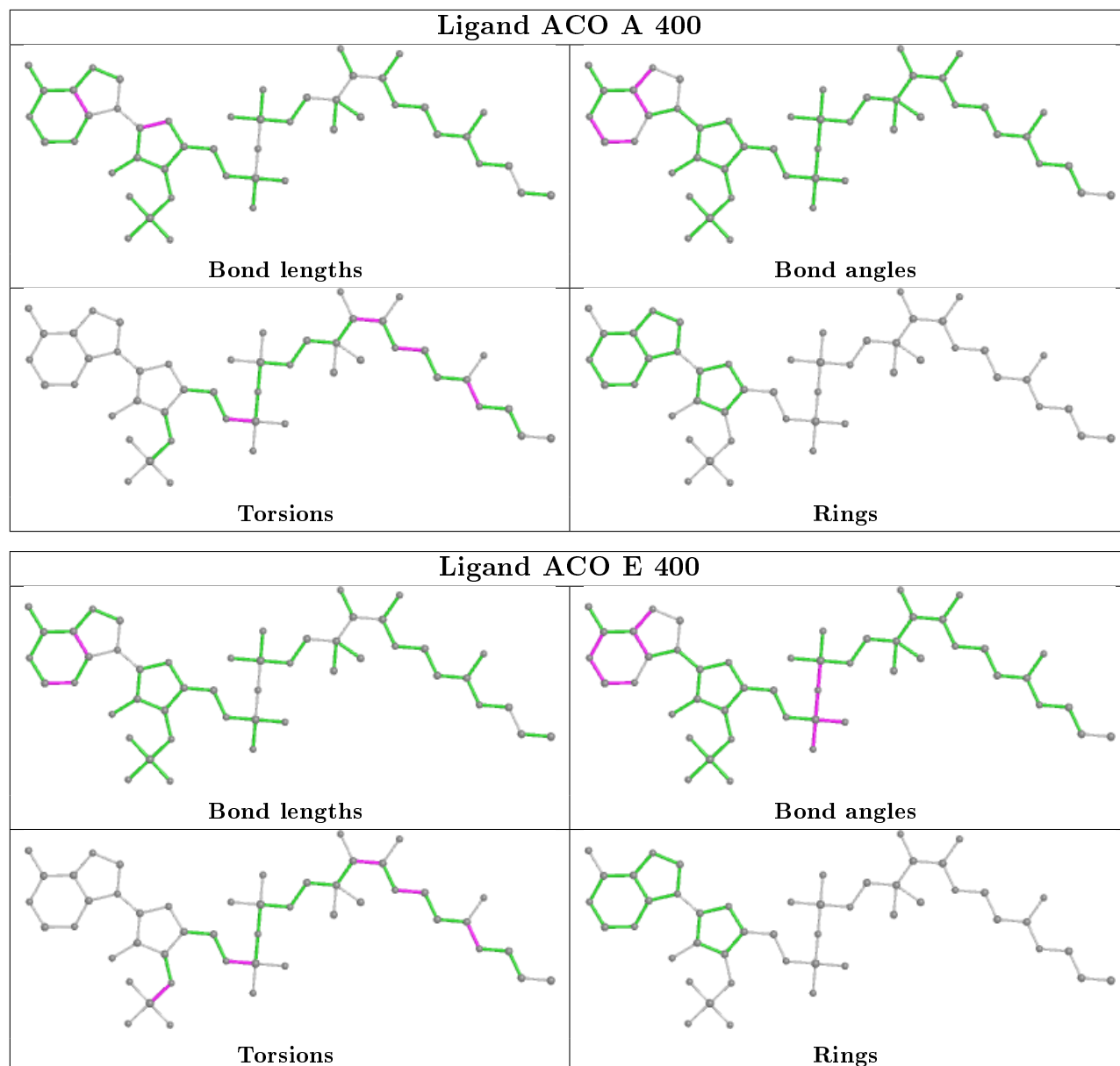
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the



average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	381/392 (97%)	-0.19	3 (0%) 86 88	17, 32, 59, 82	0
1	B	381/392 (97%)	-0.22	2 (0%) 91 92	15, 32, 58, 79	0
1	C	387/392 (98%)	-0.28	0 100 100	18, 31, 54, 72	0
1	D	381/392 (97%)	-0.04	8 (2%) 63 68	20, 41, 69, 92	0
1	E	381/392 (97%)	-0.02	9 (2%) 59 64	18, 40, 68, 87	0
1	F	382/392 (97%)	-0.33	5 (1%) 77 80	17, 33, 59, 83	0
All	All	2293/2352 (97%)	-0.18	27 (1%) 79 82	15, 34, 62, 92	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	335	GLY	5.2
1	D	30	ALA	5.1
1	D	31	ALA	4.7
1	E	334	SER	3.9
1	B	332	ASP	3.6
1	E	57	ASP	3.5
1	E	332	ASP	3.4
1	E	153	ARG	3.3
1	E	336	ASP	3.3
1	D	334	SER	3.2
1	D	57	ASP	3.2
1	E	4	ASP	3.1
1	D	332	ASP	2.9
1	F	335	GLY	2.8
1	F	334	SER	2.6
1	F	336	ASP	2.6
1	B	334	SER	2.5
1	A	57	ASP	2.5
1	F	332	ASP	2.5

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	E	337	VAL	2.4
1	F	199	GLU	2.3
1	D	39	ARG	2.3
1	E	58	GLU	2.2
1	D	34	ARG	2.2
1	A	30	ALA	2.1
1	A	31	ALA	2.0
1	D	370	SER	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](#)

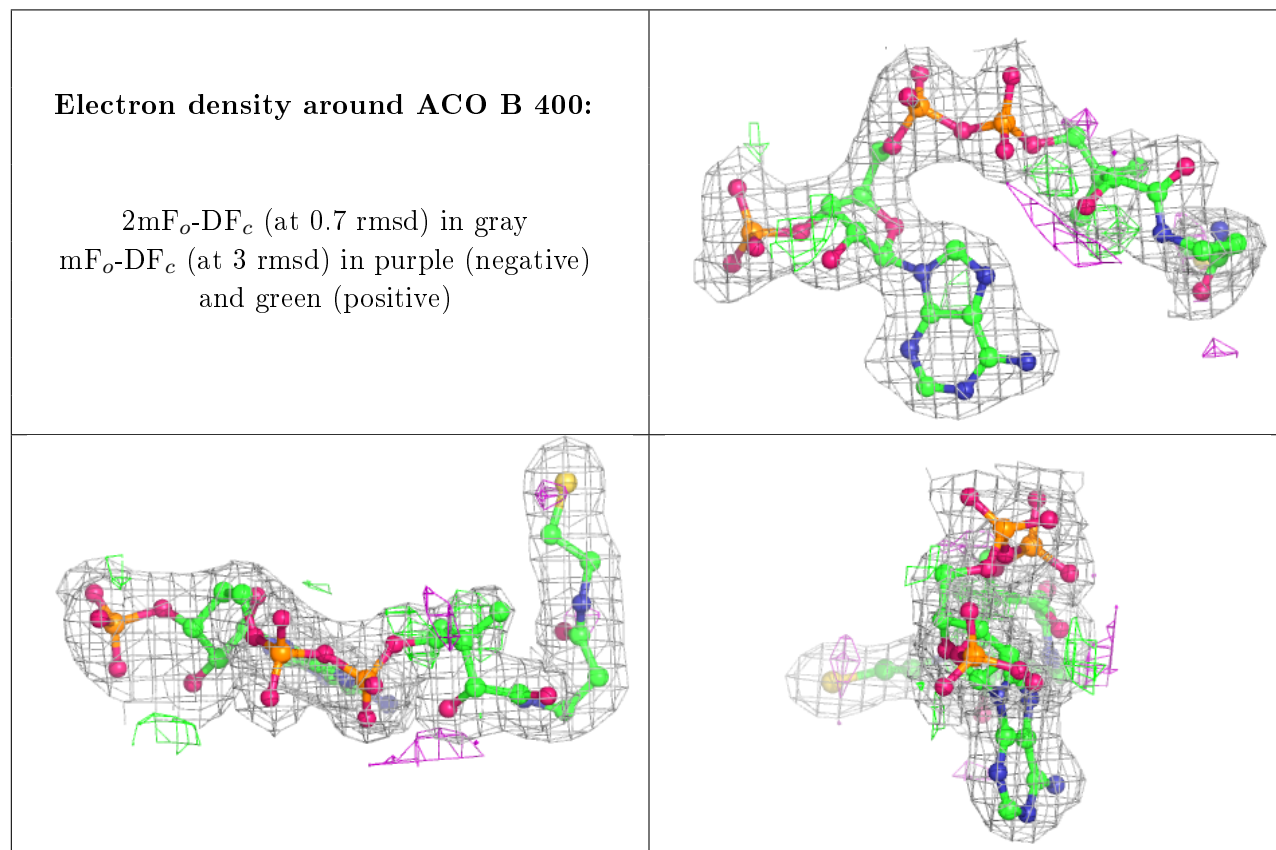
There are no carbohydrates in this entry.

## 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.

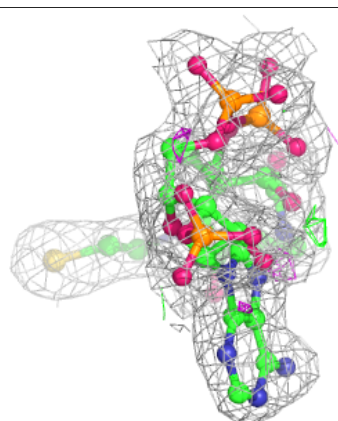
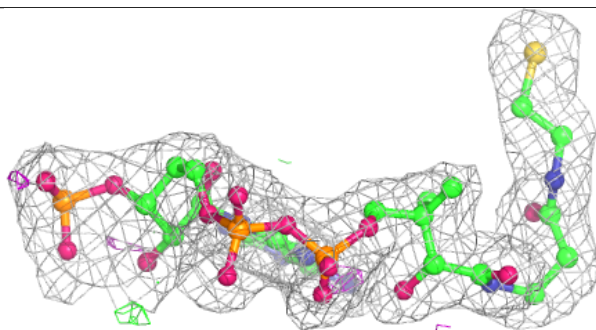
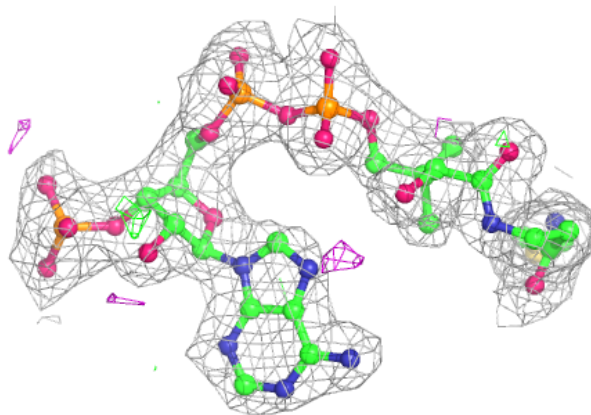
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	E	402	6/6	0.52	0.32	74,77,80,81	0
4	GOL	A	402	6/6	0.85	0.22	50,53,55,55	0
3	TRS	D	401	8/8	0.94	0.08	28,32,34,35	0
3	TRS	C	401	8/8	0.94	0.09	19,20,25,26	0
3	TRS	A	401	8/8	0.95	0.10	23,25,31,32	0
3	TRS	E	401	8/8	0.96	0.11	22,29,31,31	0
2	ACO	B	400	48/51	0.97	0.09	22,29,45,48	0
3	TRS	B	401	8/8	0.97	0.10	15,19,24,27	0
2	ACO	E	400	48/51	0.97	0.08	22,34,63,66	0
2	ACO	F	400	48/51	0.97	0.08	15,24,50,51	0
3	TRS	F	401	8/8	0.98	0.08	18,21,24,24	0
2	ACO	A	400	48/51	0.98	0.09	21,27,44,46	0
5	AC8	C	400	52/52	0.98	0.11	14,23,70,72	0
2	ACO	D	400	48/51	0.98	0.09	24,33,56,60	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.

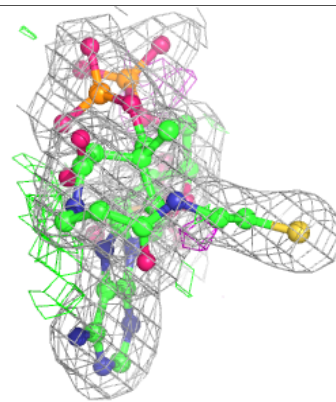
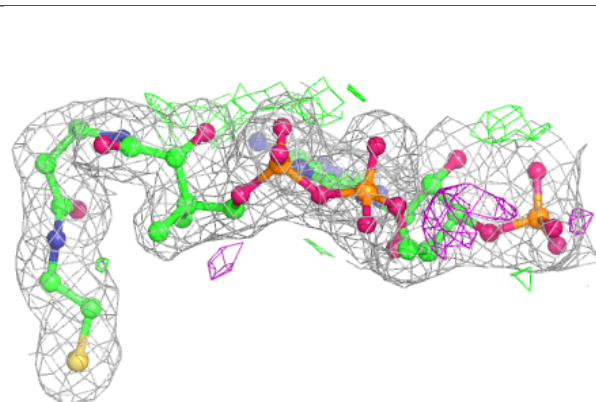
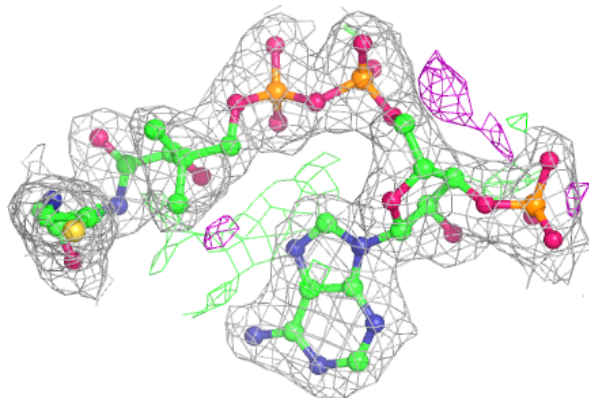


**Electron density around ACO E 400:**

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

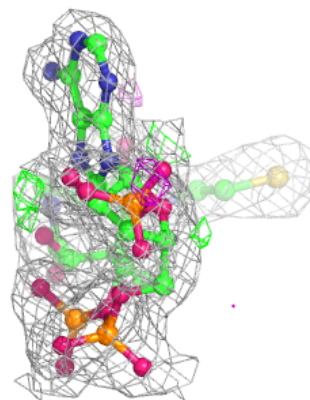
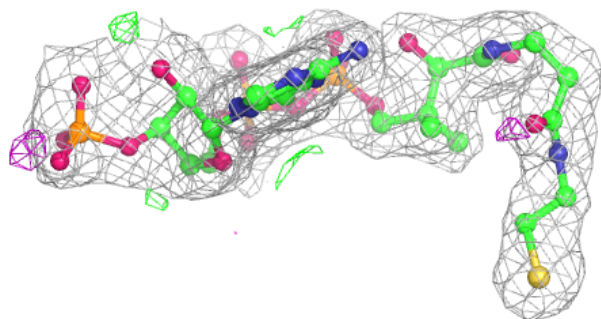
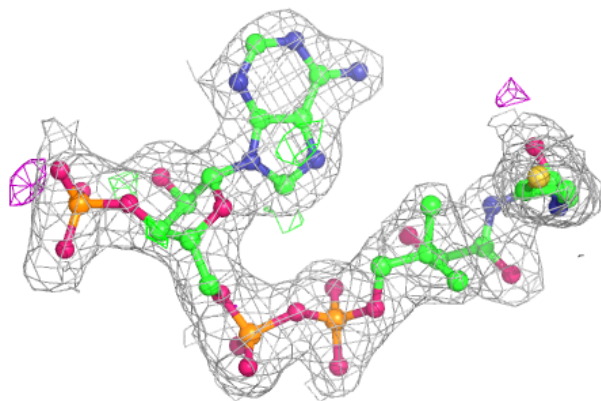
**Electron density around ACO F 400:**

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



**Electron density around ACO A 400:**

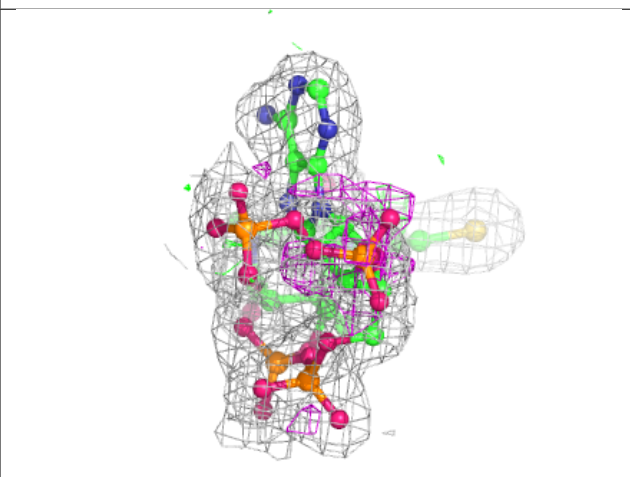
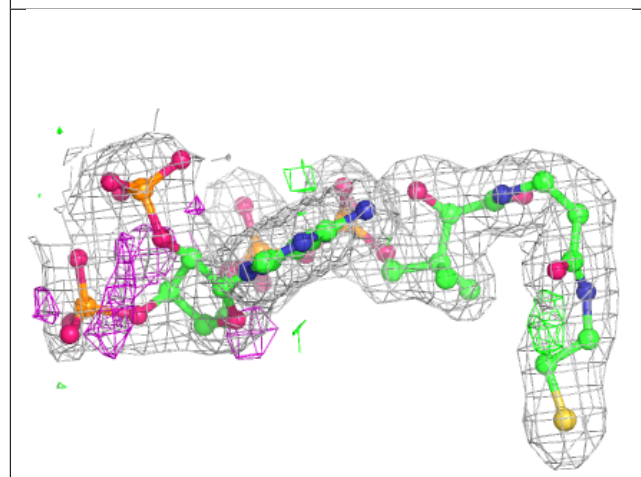
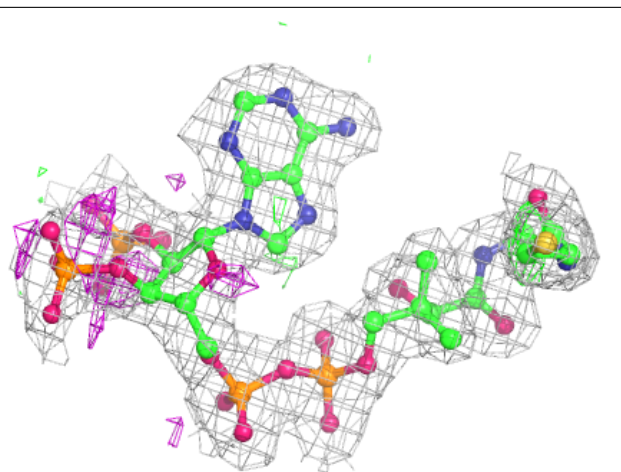
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

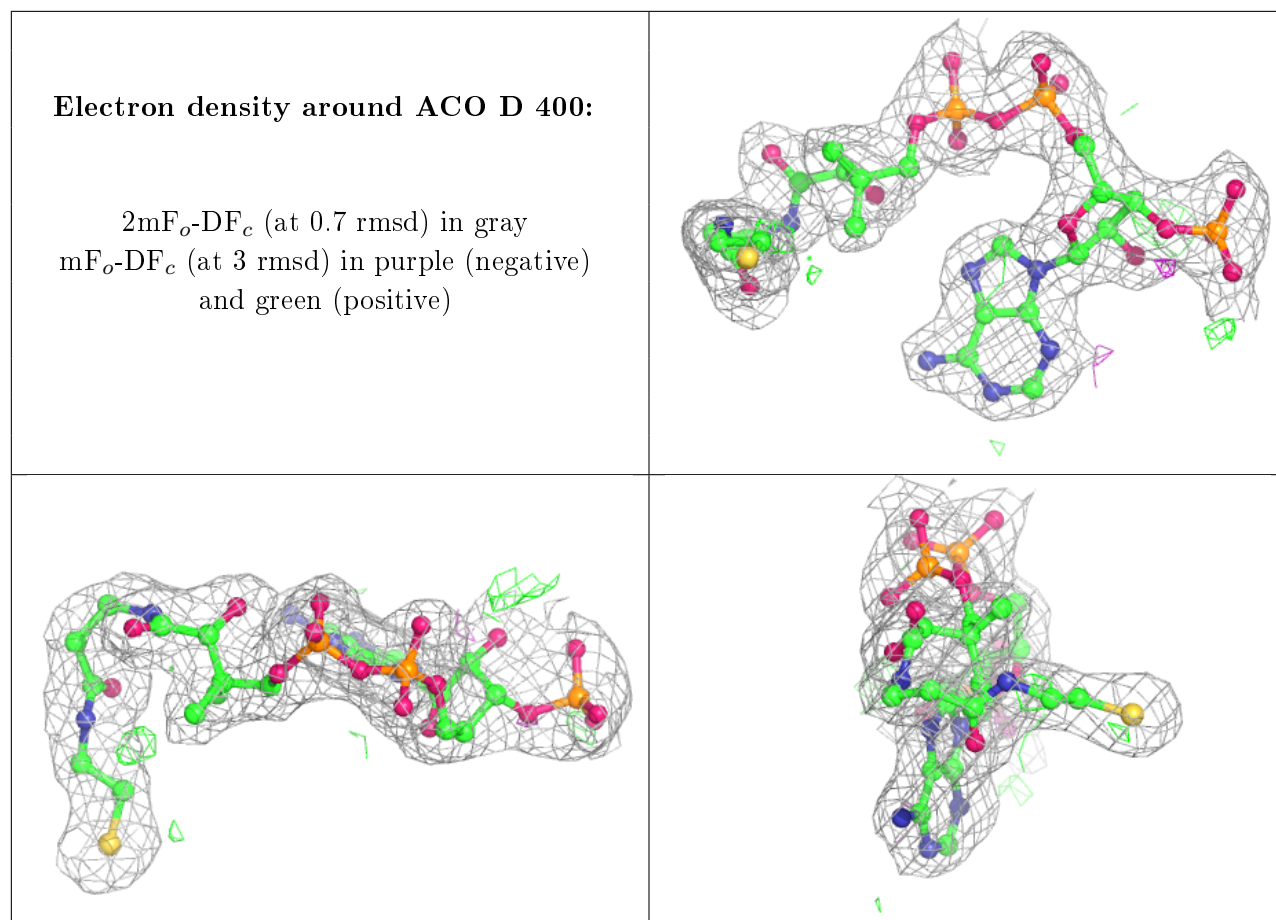




**Electron density around AC8 C 400:**

$2mF_o-DF_c$  (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.