



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2024 – 06:24 PM EDT

PDB ID : 4N6B
Title : Soybean Serine Acetyltransferase Complexed with CoA
Authors : Yi, H.; Dey, S.; Kumaran, S.; Krishnan, H.B.; Jez, J.M.
Deposited on : 2013-10-11
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.37.1
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) : 2.37.1

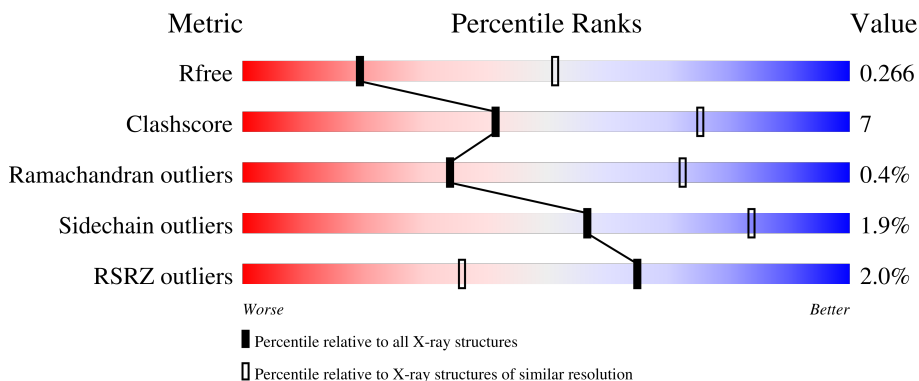
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 $\leq 5\%$. 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	286	 66% 14% 19%
1	B	286	 2% 69% 13% 17%
1	C	286	 64% 16% 19%
1	D	286	 62% 19% 19%
1	E	286	 2% 71% 11% 17%

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Mol	Chain	Length	Quality of chain
1	F	286	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into four segments: a small red segment at the beginning labeled '2%', a large green segment labeled '68%', a yellow segment labeled '12%', and a grey segment at the end labeled '19%'. A small black dot is located on the boundary between the yellow and grey segments.</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10765 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 Serine Acetyltransferase Apoenzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	233	Total 1747	C 1104	N 324	O 316	S 3	0	0	0
1	B	236	Total 1770	C 1118	N 327	O 321	S 4	0	0	0
1	C	233	Total 1753	C 1108	N 324	O 318	S 3	0	0	0
1	D	232	Total 1743	C 1102	N 323	O 315	S 3	0	0	0
1	E	237	Total 1772	C 1120	N 328	O 320	S 4	0	0	0
1	F	232	Total 1740	C 1099	N 323	O 315	S 3	0	0	0

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	LYS	SEE REMARK 999	UNP I1KHY6
A	11	LEU	SER	SEE REMARK 999	UNP I1KHY6
A	16	GLU	ASP	SEE REMARK 999	UNP I1KHY6
A	17	GLU	GLN	SEE REMARK 999	UNP I1KHY6
A	20	VAL	LEU	SEE REMARK 999	UNP I1KHY6
A	22	GLY	THR	SEE REMARK 999	UNP I1KHY6
A	34	SER	LEU	SEE REMARK 999	UNP I1KHY6
A	53	GLU	VAL	SEE REMARK 999	UNP I1KHY6
A	84	SER	PHE	SEE REMARK 999	UNP I1KHY6
A	89	ARG	CYS	SEE REMARK 999	UNP I1KHY6
A	137	ARG	GLN	SEE REMARK 999	UNP I1KHY6
A	149	ASN	ASP	SEE REMARK 999	UNP I1KHY6
A	244	ARG	GLN	SEE REMARK 999	UNP I1KHY6
B	7	ALA	LYS	SEE REMARK 999	UNP I1KHY6
B	11	LEU	SER	SEE REMARK 999	UNP I1KHY6
B	16	GLU	ASP	SEE REMARK 999	UNP I1KHY6
B	17	GLU	GLN	SEE REMARK 999	UNP I1KHY6

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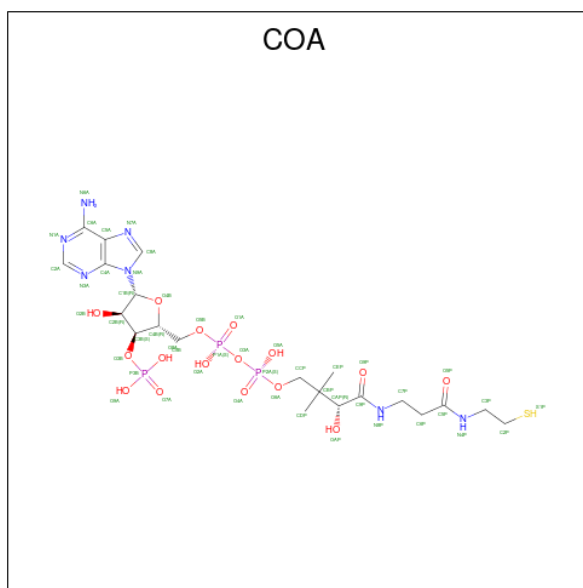
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	VAL	LEU	SEE REMARK 999	UNP I1KHY6
B	22	GLY	THR	SEE REMARK 999	UNP I1KHY6
B	34	SER	LEU	SEE REMARK 999	UNP I1KHY6
B	53	GLU	VAL	SEE REMARK 999	UNP I1KHY6
B	84	SER	PHE	SEE REMARK 999	UNP I1KHY6
B	89	ARG	CYS	SEE REMARK 999	UNP I1KHY6
B	137	ARG	GLN	SEE REMARK 999	UNP I1KHY6
B	149	ASN	ASP	SEE REMARK 999	UNP I1KHY6
B	244	ARG	GLN	SEE REMARK 999	UNP I1KHY6
C	7	ALA	LYS	SEE REMARK 999	UNP I1KHY6
C	11	LEU	SER	SEE REMARK 999	UNP I1KHY6
C	16	GLU	ASP	SEE REMARK 999	UNP I1KHY6
C	17	GLU	GLN	SEE REMARK 999	UNP I1KHY6
C	20	VAL	LEU	SEE REMARK 999	UNP I1KHY6
C	22	GLY	THR	SEE REMARK 999	UNP I1KHY6
C	34	SER	LEU	SEE REMARK 999	UNP I1KHY6
C	53	GLU	VAL	SEE REMARK 999	UNP I1KHY6
C	84	SER	PHE	SEE REMARK 999	UNP I1KHY6
C	89	ARG	CYS	SEE REMARK 999	UNP I1KHY6
C	137	ARG	GLN	SEE REMARK 999	UNP I1KHY6
C	149	ASN	ASP	SEE REMARK 999	UNP I1KHY6
C	244	ARG	GLN	SEE REMARK 999	UNP I1KHY6
D	7	ALA	LYS	SEE REMARK 999	UNP I1KHY6
D	11	LEU	SER	SEE REMARK 999	UNP I1KHY6
D	16	GLU	ASP	SEE REMARK 999	UNP I1KHY6
D	17	GLU	GLN	SEE REMARK 999	UNP I1KHY6
D	20	VAL	LEU	SEE REMARK 999	UNP I1KHY6
D	22	GLY	THR	SEE REMARK 999	UNP I1KHY6
D	34	SER	LEU	SEE REMARK 999	UNP I1KHY6
D	53	GLU	VAL	SEE REMARK 999	UNP I1KHY6
D	84	SER	PHE	SEE REMARK 999	UNP I1KHY6
D	89	ARG	CYS	SEE REMARK 999	UNP I1KHY6
D	137	ARG	GLN	SEE REMARK 999	UNP I1KHY6
D	149	ASN	ASP	SEE REMARK 999	UNP I1KHY6
D	244	ARG	GLN	SEE REMARK 999	UNP I1KHY6
E	7	ALA	LYS	SEE REMARK 999	UNP I1KHY6
E	11	LEU	SER	SEE REMARK 999	UNP I1KHY6
E	16	GLU	ASP	SEE REMARK 999	UNP I1KHY6
E	17	GLU	GLN	SEE REMARK 999	UNP I1KHY6
E	20	VAL	LEU	SEE REMARK 999	UNP I1KHY6
E	22	GLY	THR	SEE REMARK 999	UNP I1KHY6
E	34	SER	LEU	SEE REMARK 999	UNP I1KHY6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	53	GLU	VAL	SEE REMARK 999	UNP I1KHY6
E	84	SER	PHE	SEE REMARK 999	UNP I1KHY6
E	89	ARG	CYS	SEE REMARK 999	UNP I1KHY6
E	137	ARG	GLN	SEE REMARK 999	UNP I1KHY6
E	149	ASN	ASP	SEE REMARK 999	UNP I1KHY6
E	244	ARG	GLN	SEE REMARK 999	UNP I1KHY6
F	7	ALA	LYS	SEE REMARK 999	UNP I1KHY6
F	11	LEU	SER	SEE REMARK 999	UNP I1KHY6
F	16	GLU	ASP	SEE REMARK 999	UNP I1KHY6
F	17	GLU	GLN	SEE REMARK 999	UNP I1KHY6
F	20	VAL	LEU	SEE REMARK 999	UNP I1KHY6
F	22	GLY	THR	SEE REMARK 999	UNP I1KHY6
F	34	SER	LEU	SEE REMARK 999	UNP I1KHY6
F	53	GLU	VAL	SEE REMARK 999	UNP I1KHY6
F	84	SER	PHE	SEE REMARK 999	UNP I1KHY6
F	89	ARG	CYS	SEE REMARK 999	UNP I1KHY6
F	137	ARG	GLN	SEE REMARK 999	UNP I1KHY6
F	149	ASN	ASP	SEE REMARK 999	UNP I1KHY6
F	244	ARG	GLN	SEE REMARK 999	UNP I1KHY6

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	A	1	48	21	7	16	3	1	0	0
2	C	1	48	21	7	16	3	1	0	0

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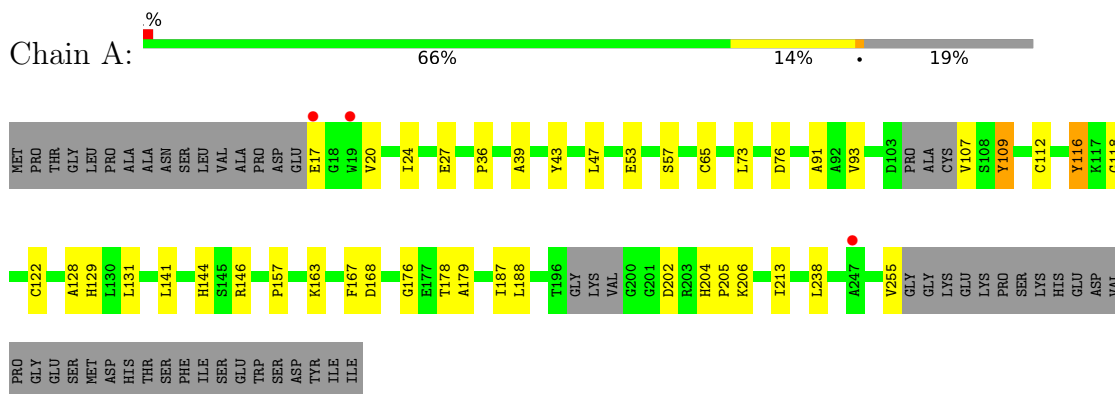
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

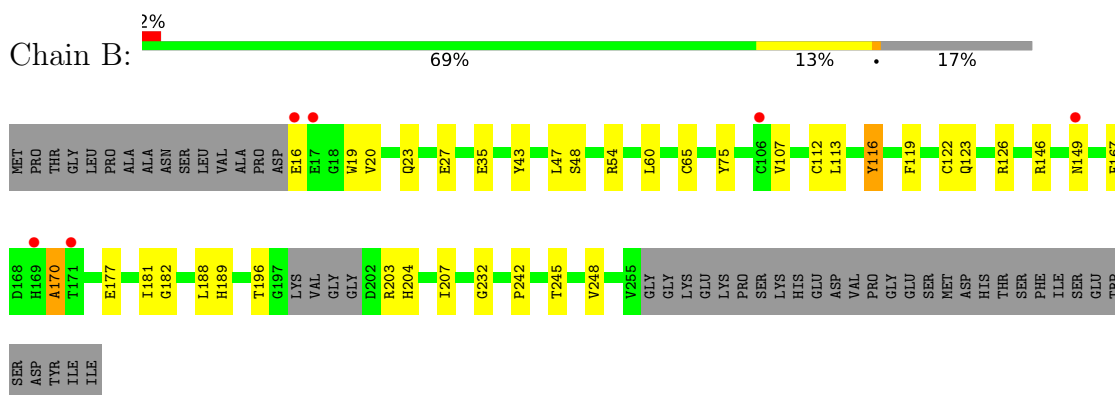
3 Residue-property plots [i](#)

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.

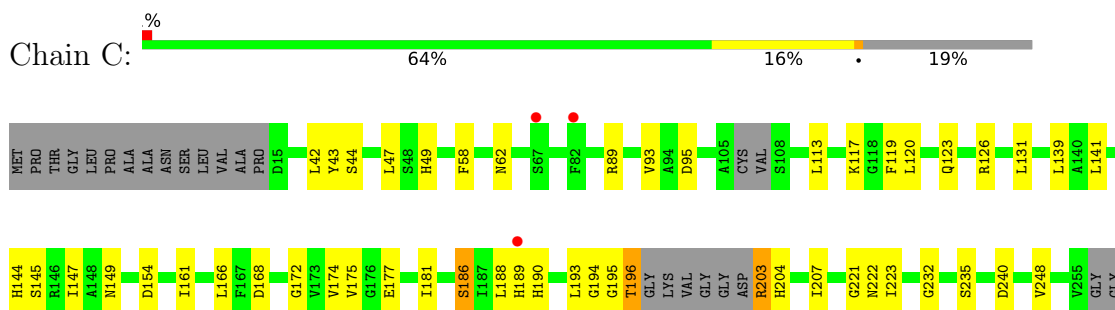
• Molecule 1: Serine Acetyltransferase Apoenzyme



• Molecule 1: Serine Acetyltransferase Apoenzyme



• Molecule 1: Serine Acetyltransferase Apoenzyme



LYS GLU
LYS LYS
SER PRO
SER LYS
HIS HIS
GLU ASP
VAL ASP
PRO VAL
GLY GLU
SER SER
MET ASP
HIS THR
SER THR
PHE PHE
ILE ILE
SER SER
GLU GLU
TRP TRP
SER SER
ASP ASP
TYR TYR
ILE ILE

● Molecule 1: Serine Acetyltransferase Apoenzyme



MET PRO THR GLY LEU PRO ALA ALA ASN SER LEU VAL GLY PRO ASP MET ASP THR HIS THR SER PHE ILE SER SER TRP TRP SER ASP TYR ILE ILE

V127 V241 L130 L131 R136 L141 H144 S145 R146 F151 A152 V153 P157 G164 D168 H169 A170 T171 G172 E177 I181 G182 N183 M184 L188 H189 H190 T196 GLY LYS VAL VAL G201 D202 R203 H204 I207 G208 D209 I219 N222 G232 V237 L238

V241 P242 V248 V255 GLY LYS LYS LYS PRO SER LYS HIS ASP VAL PRO GLY GLU MET ASP HIS THR SER PHE ILE SER SER TRP ASP TYR ILE ILE

● Molecule 1: Serine Acetyltransferase Apoenzyme



MET PRO THR GLY LEU PRO ALA ALA ASN SER LEU VAL ALA PRO ASP MET ASP THR HIS THR SER PHE ILE SER SER TRP TRP SER ASP TYR ILE ILE

T171 V174 V175 I181 L188 T196 V199 D202 K206 I207 N222 L238 P242 V248 R253 L254 V255 GLY LYS GLU LYS PRO SER LYS HIS ASP VAL PRO GLU GLU Y107 S108 Y109 Y116 F119 C122 Q123 R126 D154 I155 I161 D168 H169 A170

ILE

● Molecule 1: Serine Acetyltransferase Apoenzyme



MET PRO THR GLY LEU PRO ALA ALA ASN SER LEU VAL ALA PRO ASP MET ASP THR HIS THR SER PHE ILE SER SER TRP TRP SER ASP TYR ILE ILE

L139 M149 G164 D168 G172 T178 S186 I187 H188 H189 H190 G195 T196 GLY LYS VAL G200 G201 D202 R203 H204 P205 K206 G221 N222 V237 V248 R253 L254 V255 GLY LYS GLU LYS PRO CYS VAL S108 Y109 F119 Q123 R126 L131 R136

THR SER PHE ILE SER GLU TRP SER ASP TYR ILE ILE

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.08Å 99.18Å 120.26Å 90.00° 117.23° 90.00°	Depositor
Resolution (Å)	37.96 – 3.00 49.59 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.1 (37.96-3.00) 81.3 (49.59-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.69 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.214 , 0.268 0.217 , 0.266	Depositor DCC
R_{free} test set	2000 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	88.5	Xtrriage
Anisotropy	0.250	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 22.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10765	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.49	0/1780	0.52	0/2415
1	B	0.47	0/1805	0.53	0/2452
1	C	0.46	0/1787	0.52	0/2426
1	D	0.47	0/1776	0.50	0/2410
1	E	0.44	0/1807	0.51	0/2455
1	F	0.44	0/1773	0.50	0/2405
All	All	0.46	0/10728	0.51	0/14563

There are no bond length outliers.

There are no bond angle outliers.

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	1747	0	1772	24	0
1	B	1770	0	1793	24	0
1	C	1753	0	1775	33	0
1	D	1743	0	1769	31	0
1	E	1772	0	1799	18	0
1	F	1740	0	1763	23	0
2	A	48	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	48	0	31	1	0
2	D	48	0	31	1	0
2	E	48	0	31	3	0
2	F	48	0	31	1	0
All	All	10765	0	10826	152	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 7.

The worst 5 of 152 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:E:206:LYS:NZ	1:E:222:ASN:OD1	2.01	0.93
1:C:95:ASP:OD2	1:C:126:ARG:NH2	2.21	0.70
1:F:102:ARG:NH1	1:F:186:SER:OG	2.25	0.70
1:E:43:TYR:HA	1:E:47:LEU:HB2	1.73	0.69
1:F:195:GLY:HA2	1:F:221:GLY:H	1.56	0.68

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	227/286 (79%)	216 (95%)	11 (5%)	0	100 100
1	B	232/286 (81%)	225 (97%)	6 (3%)	1 (0%)	34 72
1	C	227/286 (79%)	218 (96%)	8 (4%)	1 (0%)	34 72
1	D	226/286 (79%)	218 (96%)	6 (3%)	2 (1%)	17 55
1	E	233/286 (82%)	221 (95%)	11 (5%)	1 (0%)	34 72
1	F	226/286 (79%)	212 (94%)	14 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1371/1716 (80%)	1310 (96%)	56 (4%)	5 (0%)	34 72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	170	ALA
1	B	170	ALA
1	D	170	ALA
1	C	222	ASN
1	D	222	ASN

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	182/226 (80%)	178 (98%)	4 (2%)	52 81
1	B	185/226 (82%)	181 (98%)	4 (2%)	52 81
1	C	183/226 (81%)	180 (98%)	3 (2%)	62 86
1	D	182/226 (80%)	177 (97%)	5 (3%)	44 77
1	E	185/226 (82%)	183 (99%)	2 (1%)	73 90
1	F	181/226 (80%)	178 (98%)	3 (2%)	60 85
All	All	1098/1356 (81%)	1077 (98%)	21 (2%)	57 84

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	202	ASP
1	E	202	ASP
1	F	248	VAL
1	F	196	THR
1	E	171	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	190	HIS
1	F	189	HIS
1	E	189	HIS
1	D	190	HIS
1	E	190	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	COA	C	700	-	41,50,50	2.32	9 (21%)	52,75,75	1.34	4 (7%)
2	COA	E	400	-	41,50,50	2.34	8 (19%)	52,75,75	1.43	7 (13%)
2	COA	D	500	-	41,50,50	2.35	8 (19%)	52,75,75	1.32	4 (7%)
2	COA	F	600	-	41,50,50	2.31	8 (19%)	52,75,75	1.45	5 (9%)
2	COA	A	300	-	41,50,50	2.34	8 (19%)	52,75,75	1.33	6 (11%)

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	COA	C	700	-	-	8/44/64/64	0/3/3/3
2	COA	E	400	-	-	6/44/64/64	0/3/3/3
2	COA	D	500	-	-	8/44/64/64	0/3/3/3
2	COA	F	600	-	-	11/44/64/64	0/3/3/3
2	COA	A	300	-	-	13/44/64/64	0/3/3/3

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	400	COA	C2B-C1B	-7.40	1.42	1.53
2	F	600	COA	C2B-C1B	-7.36	1.42	1.53
2	D	500	COA	C2B-C1B	-7.29	1.42	1.53
2	C	700	COA	C2B-C1B	-7.14	1.42	1.53
2	A	300	COA	C2B-C1B	-6.82	1.43	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	600	COA	N3A-C2A-N1A	-5.49	120.10	128.68
2	D	500	COA	N3A-C2A-N1A	-5.42	120.21	128.68
2	C	700	COA	N3A-C2A-N1A	-5.35	120.31	128.68
2	E	400	COA	N3A-C2A-N1A	-5.33	120.35	128.68
2	A	300	COA	N3A-C2A-N1A	-5.32	120.36	128.68

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

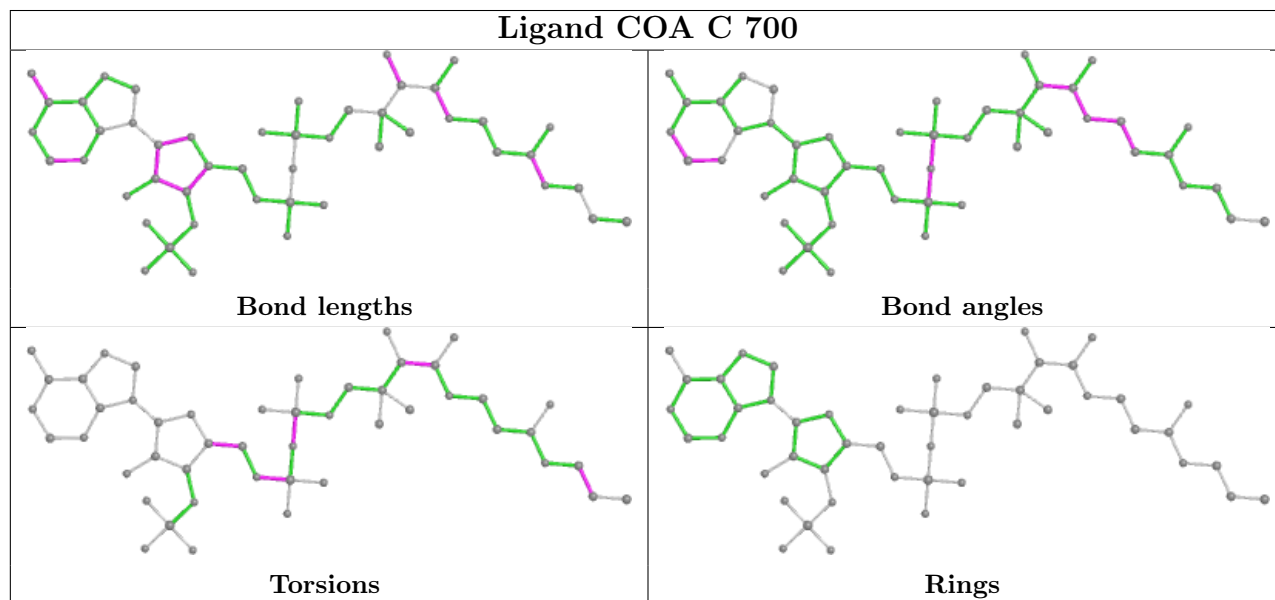
Mol	Chain	Res	Type	Atoms
2	A	300	COA	C4B-C3B-O3B-P3B
2	A	300	COA	C3B-C4B-C5B-O5B
2	A	300	COA	O4B-C4B-C5B-O5B
2	A	300	COA	C5B-O5B-P1A-O3A
2	A	300	COA	C5P-C6P-C7P-N8P

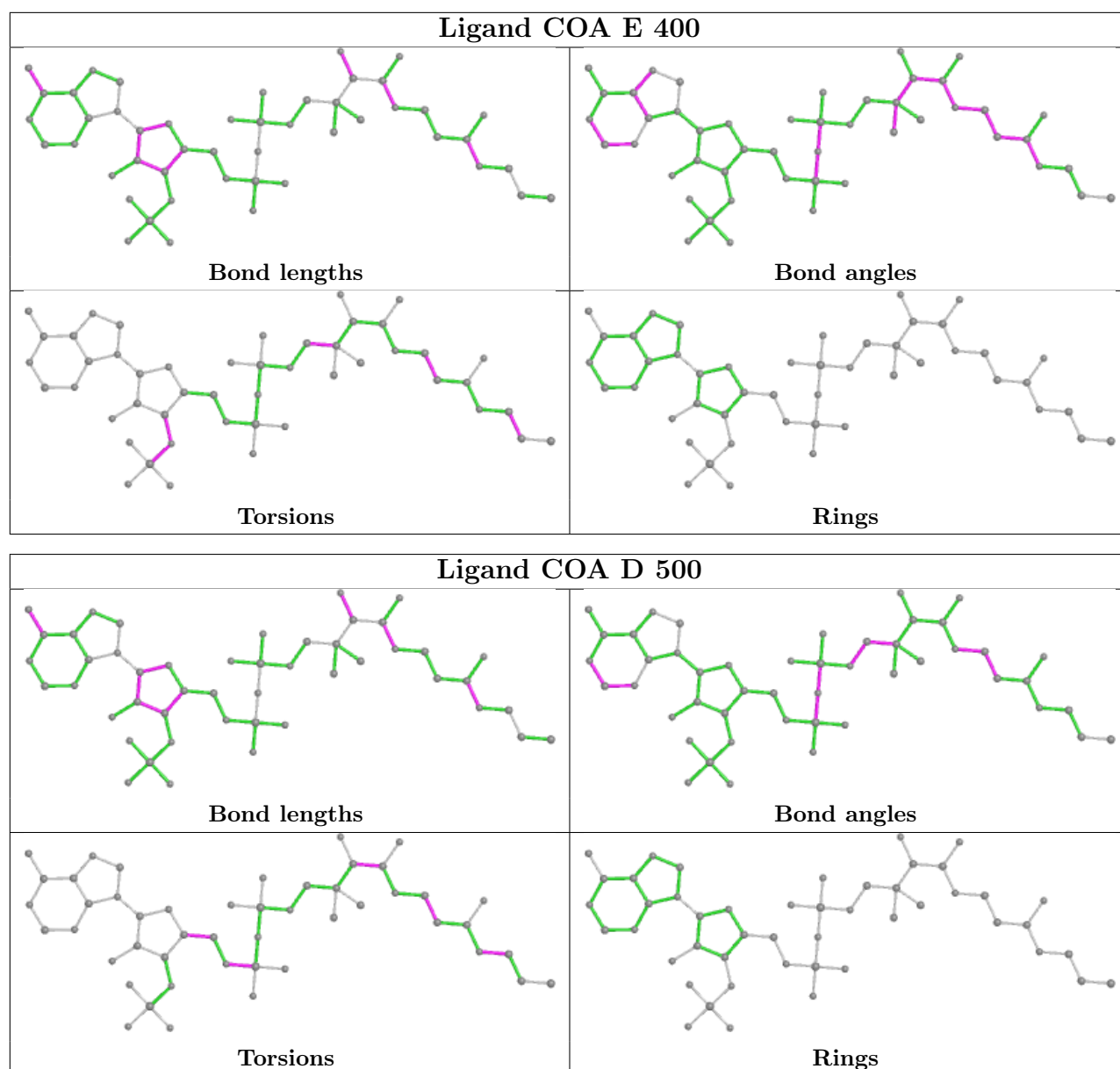
There are no ring outliers.

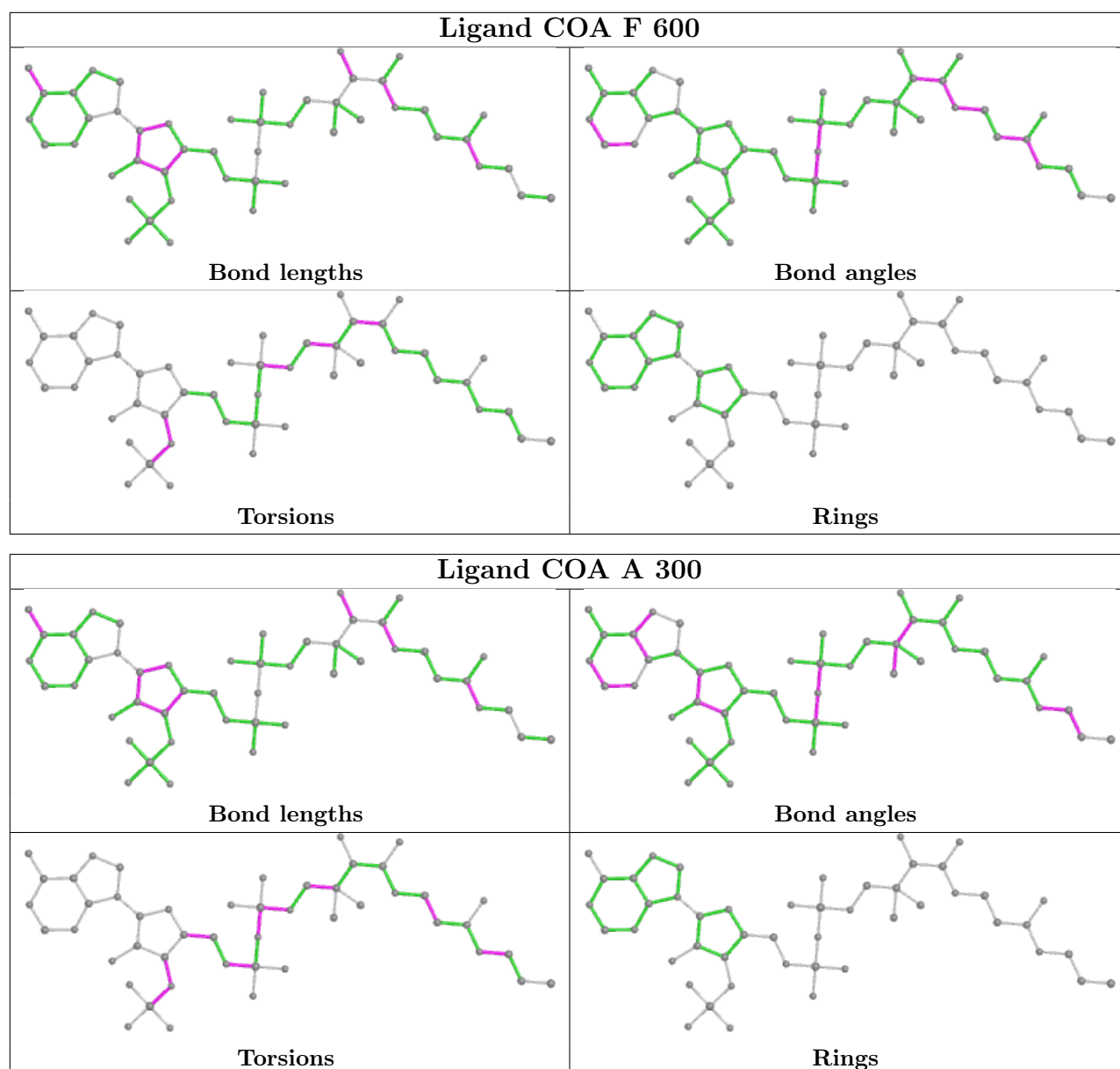
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	700	COA	1	0
2	E	400	COA	3	0
2	D	500	COA	1	0
2	F	600	COA	1	0
2	A	300	COA	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 [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	233/286 (81%)	-0.03	3 (1%) 77 51	31, 54, 89, 153	0
1	B	236/286 (82%)	-0.04	6 (2%) 57 29	34, 67, 110, 187	0
1	C	233/286 (81%)	-0.14	3 (1%) 77 51	33, 62, 93, 113	0
1	D	232/286 (81%)	-0.08	3 (1%) 77 51	34, 64, 94, 133	0
1	E	237/286 (82%)	0.04	7 (2%) 50 22	34, 64, 103, 154	0
1	F	232/286 (81%)	-0.11	6 (2%) 56 27	36, 69, 100, 120	0
All	All	1403/1716 (81%)	-0.06	28 (1%) 65 36	31, 64, 99, 187	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	109	TYR	4.0
1	F	17	GLU	3.7
1	E	104	PRO	3.0
1	B	106	CYS	2.9
1	D	19	TRP	2.9

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

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

6.3 Carbohydrates [i](#)

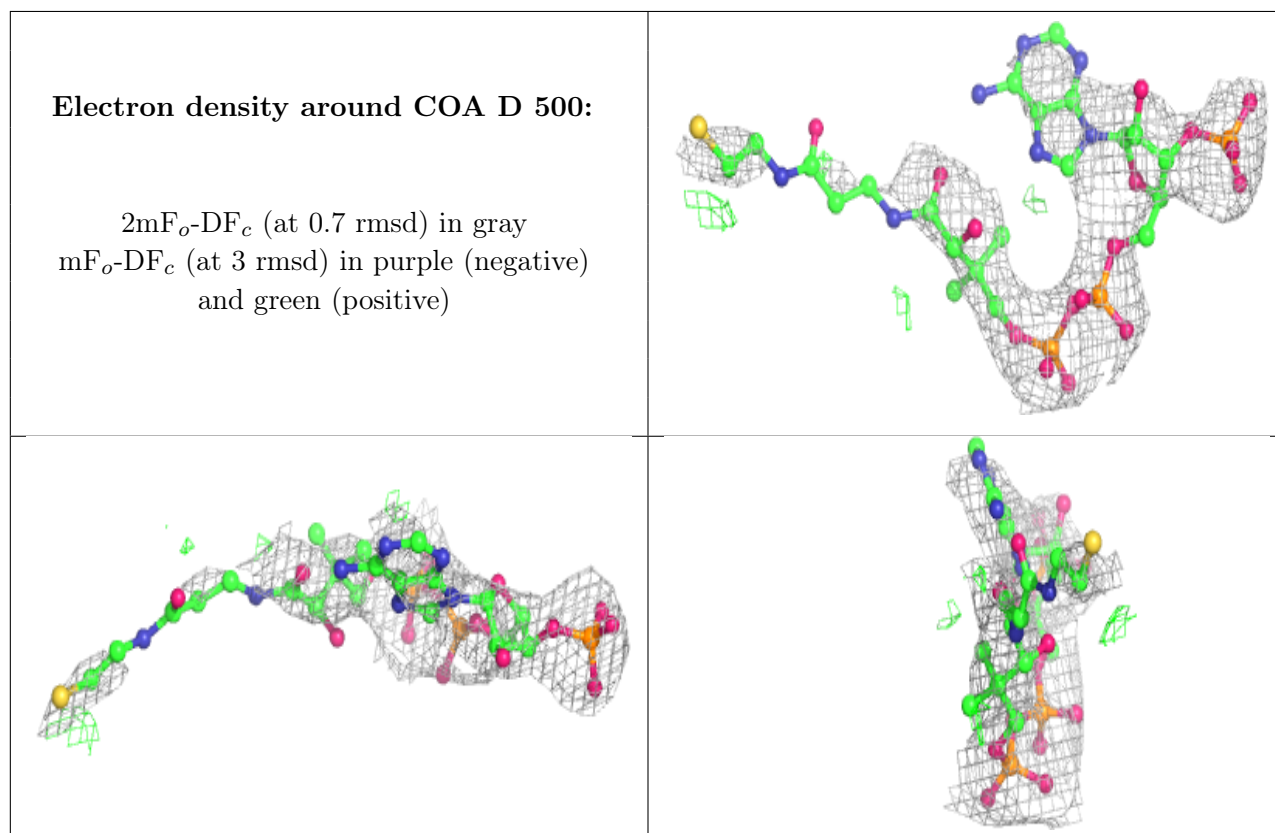
There are no monosaccharides in this entry.

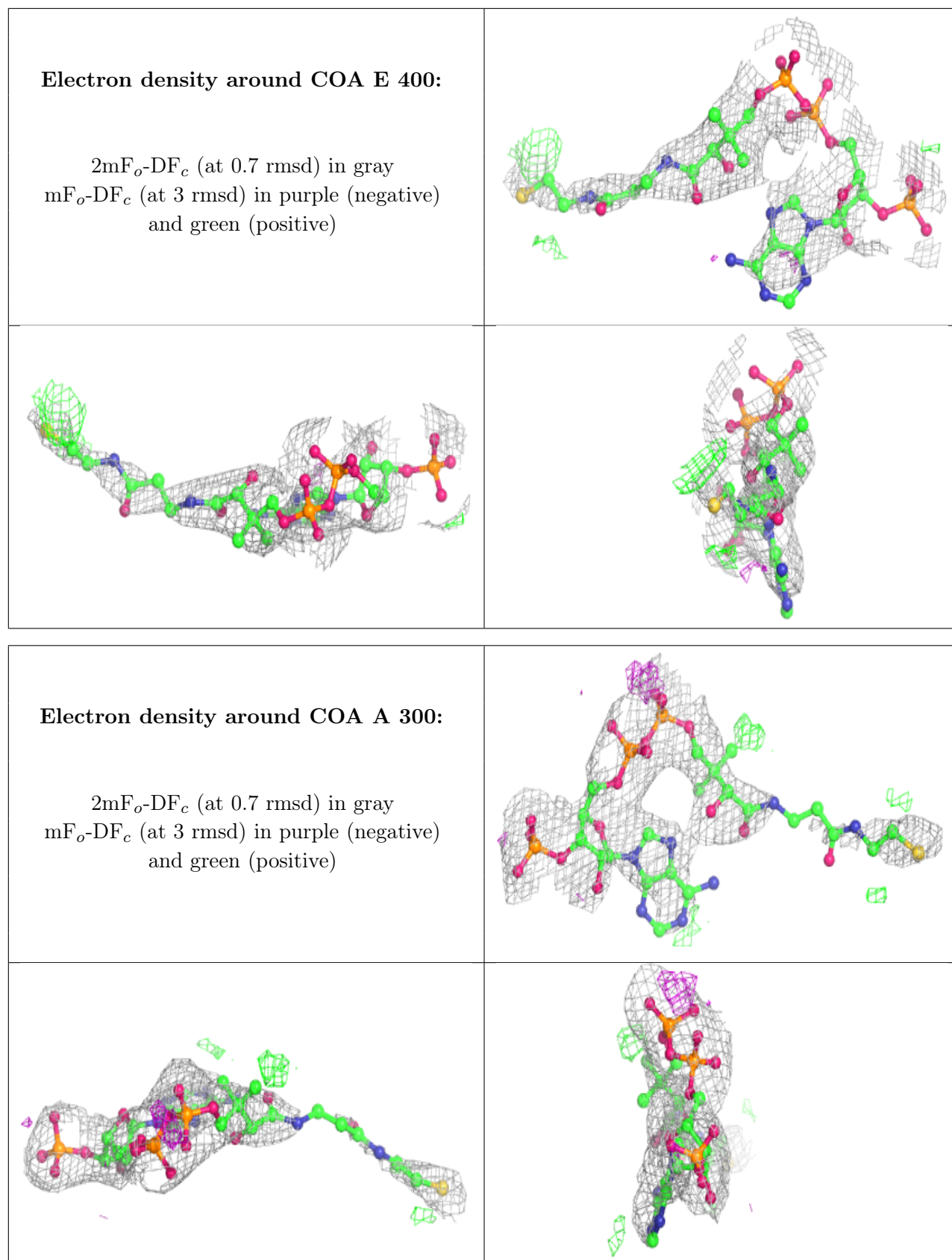
6.4 Ligands [i](#)

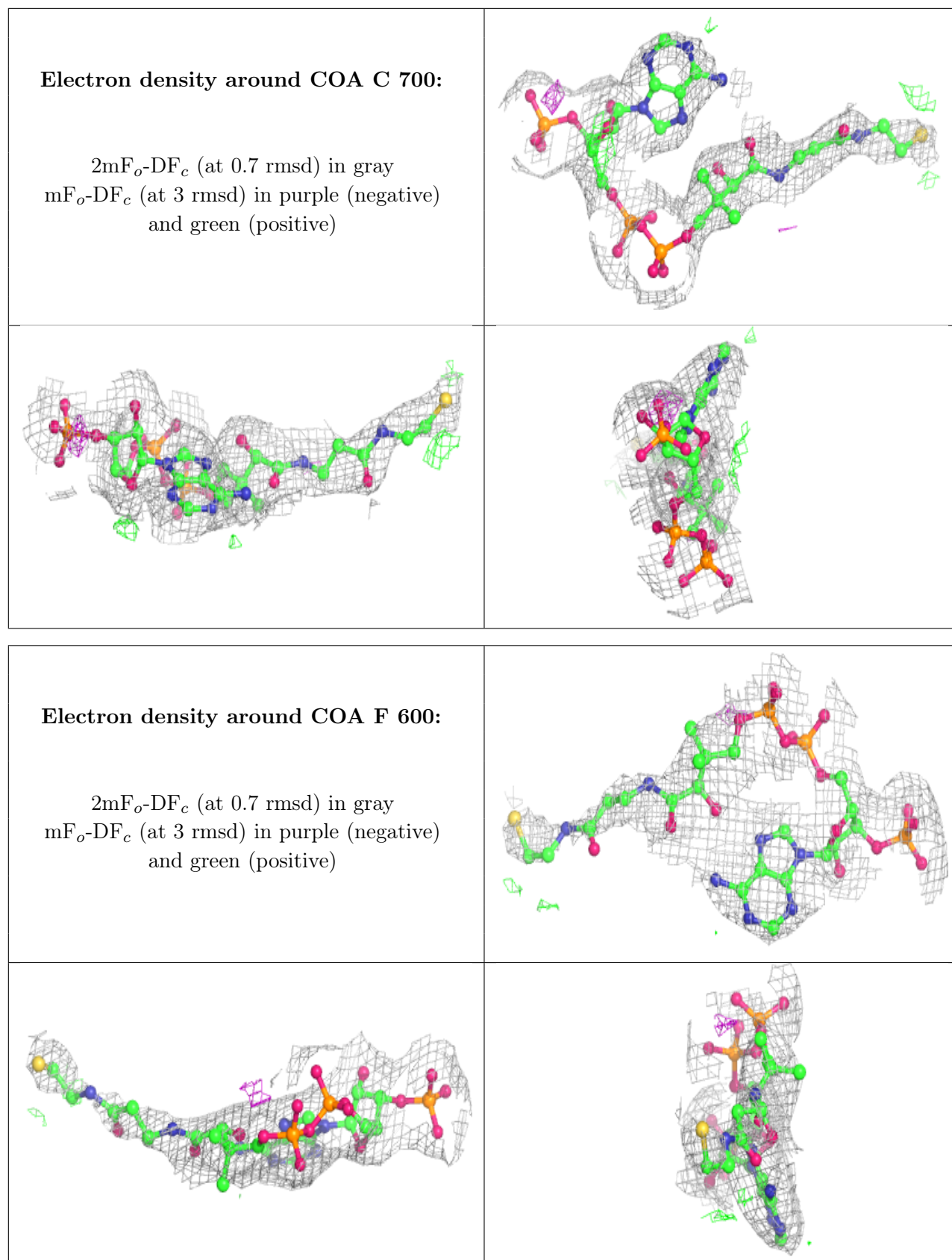
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	COA	D	500	48/48	0.80	0.44	62,129,158,283	0
2	COA	E	400	48/48	0.87	0.27	52,94,125,233	0
2	COA	A	300	48/48	0.88	0.33	67,105,128,226	48
2	COA	C	700	48/48	0.90	0.18	53,94,117,171	0
2	COA	F	600	48/48	0.92	0.16	61,92,132,198	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







6.5 Other polymers [i](#)

There are no such residues in this entry.