



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:46 AM UTC

PDB ID : 4N6B / pdb_00004n6b
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

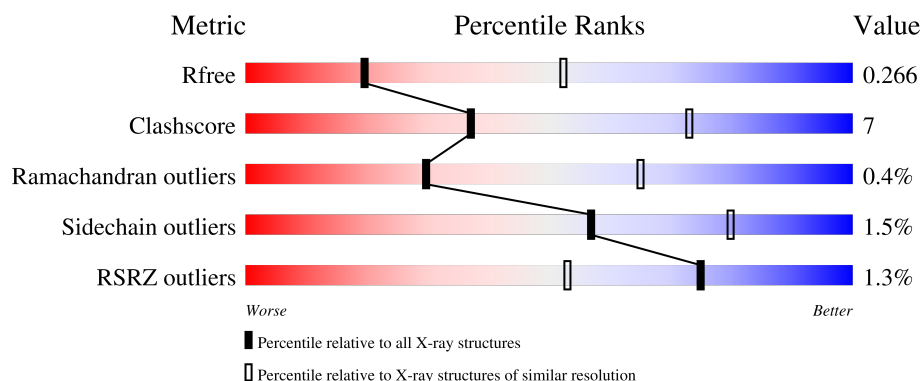
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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	
1	B	286	
1	C	286	
1	D	286	
1	E	286	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	286	% 67%13%19%

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

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

Continued on next page...

Continued from previous page...

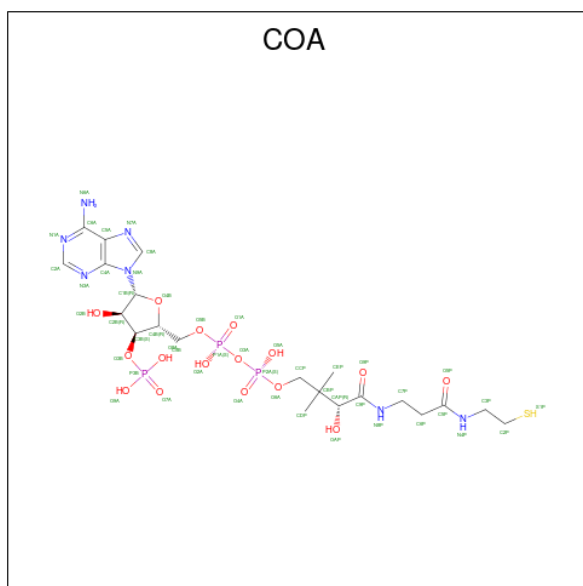
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	VAL	LEU	SEE REMARK 999	UNP I1KHY6
B	22	GLY	THR	SEE REMARK 999	UNP I1KHY6
B	34	SER	LEU	SEE REMARK 999	UNP I1KHY6
B	53	GLU	VAL	SEE REMARK 999	UNP I1KHY6
B	84	SER	PHE	SEE REMARK 999	UNP I1KHY6
B	89	ARG	CYS	SEE REMARK 999	UNP I1KHY6
B	137	ARG	GLN	SEE REMARK 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

Continued on next page...

Continued from previous page...

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 (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

Continued on next page...

Continued from previous page...

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		

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

● Molecule 1: Serine Acetyltransferase Apoenzyme

Chain D: 2% 62% 18% 19%

MET PRO THR GLY LEU PRO ALA ALA ASN SER LEU VAL PRO GLY ASP MET GLU E17 G18 G19 E27 Y43 Y46 L47 R54 T72 D76 L77 F78 L79 D85 P86 S87 D95 R100 E101 R102 D103 PRO ALA CYS V107 S108 Y109 L113 F119 Q123 R126

V127 L130 L131 R136 L141 R146 F151 A152 V153 P157 G164 D168 H169 A170 T171 G172 E177 I181 G182 N183 M184 L188 H189 H190 T196 GLY LYS VAL GLY G201 D202 R203 H204 T207 G208 D209 I219 N222 G232 V237 L238 V241

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

● Molecule 1: Serine Acetyltransferase Apoenzyme

Chain E: 72% 11% 17%

MET PRO THR GLY LEU PRO ALA ALA ASN SER LEU VAL PRO GLY ASP MET GLU E17 E35 P36 Y43 L47 F58 N62 L70 D95 P104 V107 Y116 F119 C122 Q123 R126 D154 I155 I161 D168 H169 A170 T171 V174 V175 I181

L188 L196 T199 K206 I207 N222 L238 P242 V248 L254 V255 GLY GLY LYS LYS PRO SER LYS HIS GLU ASP VAL PRO GLY SER MET ASP HIS THR SER PHE ILE SER GLU TRP SER ASP TYR ILE ILE

● Molecule 1: Serine Acetyltransferase Apoenzyme

Chain F: 67% 13% 19%

MET PRO THR GLY LEU PRO ALA ALA ASN SER LEU VAL PRO GLY ASP MET GLU E17 T24 P36 A39 L42 Y43 L47 E53 D85 P86 S87 L88 R89 S90 A91 V93 A94 D95 A98 R102 D103 PRO ALA CYS VAL S108 Y109 F119 Q123 R126

L131 R136 L139 G164 D168 G172 T178 S186 I187 L188 H189 H190 G195 T196 GLY LYS VAL G200 G201 D202 R203 H204 P205 K206 G221 N222 T239 V248 V255 GLY GLY LYS GLU LYS PRO SER LYS HIS GLU ASP VAL PRO GLY SER MET ASP HIS

THR SER PHE ILE SER GLU TRP SER ASP TYR 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 37.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (37.96-3.00) 81.2 (37.96-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.69 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.214 , 0.268 0.216 , 0.266	Depositor DCC
R_{free} test set	2000 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å ²)	88.5	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10765	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

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	0.69	0/1780	0.84	0/2415
1	B	0.67	0/1805	0.89	0/2452
1	C	0.66	0/1787	0.90	5/2426 (0.2%)
1	D	0.66	0/1776	0.83	2/2410 (0.1%)
1	E	0.64	0/1807	0.88	0/2455
1	F	0.62	0/1773	0.85	2/2405 (0.1%)
All	All	0.66	0/10728	0.87	9/14563 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	VAL	CA-C-N	8.48	125.85	119.66
1	C	241	VAL	C-N-CA	8.48	125.85	119.66
1	C	103	ASP	CA-C-N	5.94	125.42	119.24
1	C	103	ASP	C-N-CA	5.94	125.42	119.24
1	C	100	ARG	N-CA-C	-5.40	106.37	113.12
1	F	85	ASP	CA-C-N	5.05	124.54	119.19
1	F	85	ASP	C-N-CA	5.05	124.54	119.19
1	D	241	VAL	CA-C-N	5.05	123.34	119.66
1	D	241	VAL	C-N-CA	5.05	123.34	119.66

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1747	0	1772	24	0
1	B	1770	0	1793	25	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	24	0
2	A	48	0	31	3	0
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	154	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.

All (154) 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
1:F:172:GLY:HA3	1:F:190:HIS:HD2	1.59	0.68
1:D:43:TYR:HA	1:D:47:LEU:HB2	1.78	0.66
1:C:194:GLY:HA3	2:F:600:COA:H22	1.80	0.64
1:E:95:ASP:OD2	1:E:126:ARG:NH2	2.30	0.63
1:C:196:THR:O	1:C:196:THR:OG1	2.13	0.63
1:A:168:ASP:HB3	1:A:188:LEU:HD22	1.81	0.62
1:C:58:PHE:O	1:C:62:ASN:ND2	2.33	0.62
1:F:204:HIS:O	1:F:206:LYS:NZ	2.32	0.61
1:A:73:LEU:HD13	1:C:44:SER:HB2	1.81	0.61
1:D:95:ASP:OD2	1:D:126:ARG:NH2	2.32	0.61
1:F:172:GLY:HA3	1:F:190:HIS:CD2	2.36	0.61
1:C:43:TYR:HA	1:C:47:LEU:HB2	1.81	0.60
1:D:172:GLY:HA3	1:D:190:HIS:HD2	1.67	0.58
1:B:113:LEU:HD12	1:B:119:PHE:HE2	1.67	0.58
1:F:102:ARG:NH2	1:F:164:GLY:O	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:CYS:O	1:A:146:ARG:NH2	2.35	0.57
1:F:196:THR:O	1:F:196:THR:OG1	2.23	0.57
1:C:168:ASP:HB3	1:C:188:LEU:HD22	1.87	0.57
1:D:78:PHE:HD1	1:D:127:VAL:HG21	1.69	0.56
1:D:183:ASN:N	1:D:209:ASP:OD1	2.25	0.56
1:B:43:TYR:HA	1:B:47:LEU:HB2	1.87	0.56
1:D:85:ASP:OD1	1:D:87:SER:OG	2.23	0.55
2:A:300:COA:O5B	2:A:300:COA:H8A	2.07	0.55
1:E:161:ILE:HG22	1:E:181:ILE:HD12	1.88	0.55
1:C:172:GLY:HA3	1:C:190:HIS:HD2	1.73	0.54
1:E:154:ASP:HB3	1:E:174:VAL:HG22	1.89	0.54
1:B:181:ILE:HA	1:B:207:ILE:HB	1.90	0.53
1:C:172:GLY:HA3	1:C:190:HIS:CD2	2.44	0.53
1:A:107:VAL:HG21	1:A:112:CYS:HB2	1.90	0.52
1:F:202:ASP:O	1:F:222:ASN:ND2	2.42	0.52
1:E:58:PHE:O	1:E:62:ASN:ND2	2.35	0.52
1:D:177:GLU:H	1:D:204:HIS:CE1	2.28	0.51
1:C:232:GLY:O	1:C:235:SER:OG	2.22	0.51
1:F:17:GLU:HB2	1:F:93:VAL:HG21	1.93	0.51
1:A:129:HIS:ND1	1:A:157:PRO:O	2.36	0.51
1:C:145:SER:O	1:C:149:ASN:ND2	2.44	0.51
1:E:122:CYS:O	1:E:126:ARG:HG3	2.11	0.51
1:A:187:ILE:HG12	1:A:213:ILE:HD12	1.94	0.50
1:D:78:PHE:CD1	1:D:127:VAL:HG21	2.46	0.50
1:E:107:VAL:HG11	1:E:116:TYR:CZ	2.47	0.50
1:B:232:GLY:HA3	1:B:248:VAL:HG23	1.94	0.50
1:C:113:LEU:O	1:C:120:LEU:HD21	2.12	0.50
1:C:144:HIS:HA	1:C:147:ILE:HD12	1.94	0.49
1:E:248:VAL:HG21	2:E:400:COA:C4A	2.42	0.49
1:A:27:GLU:OE1	1:A:109:TYR:N	2.45	0.49
1:F:102:ARG:HH11	1:F:186:SER:HG	1.60	0.49
1:B:182:GLY:N	1:B:207:ILE:O	2.42	0.49
1:A:118:GLY:HA3	1:A:167:PHE:HB2	1.95	0.49
1:D:102:ARG:NH2	1:D:164:GLY:O	2.43	0.49
1:B:149:ASN:OD1	1:C:117:LYS:HE3	2.13	0.48
1:D:172:GLY:HA3	1:D:190:HIS:CD2	2.46	0.48
1:D:146:ARG:HA	1:D:146:ARG:HD2	1.62	0.48
1:D:238:LEU:HD11	2:E:400:COA:C5A	2.43	0.48
1:D:169:HIS:O	1:D:171:THR:N	2.47	0.48
1:F:95:ASP:OD2	1:F:123:GLN:NE2	2.47	0.47
1:C:154:ASP:HB3	1:C:174:VAL:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HA	1:A:144:HIS:HB3	1.96	0.47
1:A:176:GLY:HA3	1:A:204:HIS:CD2	2.50	0.47
1:C:166:LEU:HB3	1:C:186:SER:HA	1.94	0.47
1:C:195:GLY:HA2	1:C:221:GLY:H	1.79	0.47
1:C:189:HIS:CE1	1:C:190:HIS:CD2	3.03	0.47
1:C:223:ILE:HB	1:C:240:ASP:OD1	2.14	0.47
1:A:76:ASP:OD2	1:C:49:HIS:NE2	2.44	0.47
1:A:238:LEU:HD11	2:D:500:COA:C5A	2.45	0.46
1:C:232:GLY:HA3	1:C:248:VAL:HG12	1.96	0.46
1:D:102:ARG:HH22	1:D:184:ASN:HA	1.80	0.46
1:B:122:CYS:O	1:B:126:ARG:HG3	2.16	0.46
1:A:53:GLU:O	1:A:57:SER:OG	2.18	0.46
1:C:203:ARG:NH2	1:C:204:HIS:HE1	2.13	0.46
1:F:98:ALA:HB1	1:F:102:ARG:NH2	2.31	0.46
1:C:161:ILE:HG22	1:C:181:ILE:HD12	1.98	0.45
1:B:113:LEU:HD12	1:B:119:PHE:CE2	2.50	0.45
1:B:54:ARG:NH2	1:D:76:ASP:OD1	2.50	0.45
1:D:131:LEU:HD22	1:D:136:ARG:HD3	1.99	0.45
1:B:242:PRO:O	1:B:245:THR:OG1	2.22	0.45
2:A:300:COA:C5A	1:E:238:LEU:HD11	2.47	0.45
1:C:119:PHE:O	1:C:123:GLN:HG2	2.16	0.45
1:C:89:ARG:O	1:C:93:VAL:HG23	2.17	0.44
1:F:36:PRO:HA	1:F:39:ALA:HB2	2.00	0.44
1:B:119:PHE:O	1:B:123:GLN:HG2	2.17	0.44
1:E:119:PHE:O	1:E:123:GLN:HG2	2.16	0.44
1:E:169:HIS:O	1:E:171:THR:N	2.50	0.44
1:B:107:VAL:HG11	1:B:116:TYR:CE1	2.52	0.44
1:B:23:GLN:O	1:B:27:GLU:HG3	2.18	0.44
1:C:131:LEU:HD22	1:C:139:LEU:HD23	2.00	0.44
1:A:36:PRO:HA	1:A:39:ALA:HB2	2.00	0.44
1:B:19:TRP:CZ3	1:B:23:GLN:HG3	2.53	0.44
1:B:167:PHE:HB3	1:B:170:ALA:HB2	1.99	0.44
1:C:175:VAL:HG13	1:C:193:LEU:HD12	2.00	0.44
1:D:46:ILE:HD11	1:D:113:LEU:HD23	1.99	0.44
1:E:168:ASP:HB3	1:E:188:LEU:HD22	2.00	0.44
1:A:112:CYS:O	1:A:116:TYR:HB2	2.18	0.44
1:B:146:ARG:HD2	1:B:146:ARG:HA	1.60	0.44
1:E:155:ILE:HG23	1:E:175:VAL:HB	2.00	0.43
1:D:100:ARG:HG2	1:D:109:TYR:CE2	2.53	0.43
1:F:43:TYR:HA	1:F:47:LEU:HB2	2.00	0.43
2:A:300:COA:H133	2:A:300:COA:N7A	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:PRO:HD2	1:E:254:LEU:HD21	2.01	0.43
1:C:181:ILE:HA	1:C:207:ILE:HB	2.00	0.43
1:F:168:ASP:HB3	1:F:188:LEU:HD22	2.00	0.43
1:B:65:CYS:O	1:B:146:ARG:NH2	2.48	0.43
1:D:119:PHE:O	1:D:123:GLN:HG2	2.19	0.43
1:E:70:LEU:HD23	1:E:70:LEU:HA	1.86	0.43
1:D:219:ILE:HG23	1:D:237:VAL:HB	2.00	0.43
1:F:85:ASP:OD1	1:F:87:SER:OG	2.34	0.43
1:A:128:ALA:HA	1:A:131:LEU:HD12	2.01	0.43
1:A:178:THR:O	1:A:206:LYS:NZ	2.51	0.43
1:B:35:GLU:HG2	1:F:139:LEU:HB2	2.01	0.43
1:F:131:LEU:HD22	1:F:136:ARG:HD3	2.01	0.42
1:C:42:LEU:HD23	1:C:42:LEU:HA	1.93	0.42
1:D:151:PHE:O	1:D:153:VAL:HG23	2.18	0.42
1:E:35:GLU:HA	1:E:36:PRO:HD2	1.87	0.42
1:A:17:GLU:HB2	1:A:93:VAL:HG21	2.01	0.42
1:A:43:TYR:HA	1:A:47:LEU:HB2	2.01	0.42
2:C:700:COA:H8A	2:C:700:COA:H2B	1.84	0.42
1:F:53:GLU:OE2	1:F:89:ARG:HD2	2.18	0.42
2:E:400:COA:H133	2:E:400:COA:N7A	2.34	0.42
1:C:203:ARG:NH2	1:C:204:HIS:CE1	2.87	0.42
1:D:141:LEU:HD23	1:D:157:PRO:HG2	2.02	0.42
1:F:178:THR:HG21	1:F:201:GLY:O	2.20	0.42
1:B:112:CYS:O	1:B:116:TYR:HB2	2.20	0.42
1:B:60:LEU:HD23	1:B:60:LEU:HA	1.88	0.41
1:F:42:LEU:HD23	1:F:42:LEU:HA	1.87	0.41
1:A:122:CYS:SG	1:A:167:PHE:CE1	3.14	0.41
1:C:141:LEU:HA	1:C:144:HIS:HB3	2.02	0.41
1:D:181:ILE:HA	1:D:207:ILE:HB	2.02	0.41
1:A:146:ARG:HA	1:A:146:ARG:HD2	1.65	0.41
1:D:168:ASP:HB3	1:D:188:LEU:HD22	2.02	0.41
1:D:232:GLY:HA3	1:D:248:VAL:HG23	2.02	0.41
1:B:16:GLU:O	1:B:20:VAL:HG23	2.21	0.41
1:B:43:TYR:CE1	1:B:48:SER:HB3	2.55	0.41
1:D:241:VAL:HA	1:D:242:PRO:HD2	1.90	0.41
1:E:181:ILE:HA	1:E:207:ILE:HB	2.03	0.41
1:F:24:ILE:HG12	1:F:109:TYR:HB3	2.02	0.41
1:F:119:PHE:O	1:F:123:GLN:HG2	2.21	0.41
1:D:95:ASP:OD2	1:D:123:GLN:NE2	2.52	0.41
1:D:141:LEU:HD23	1:D:141:LEU:HA	1.90	0.41
1:B:40:SER:O	1:B:44:SER:OG	2.31	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:GLU:OE1	1:D:109:TYR:HD1	2.04	0.41
1:C:189:HIS:NE2	1:C:190:HIS:CE1	2.89	0.40
1:A:20:VAL:O	1:A:24:ILE:HG13	2.22	0.40
1:A:91:ALA:HA	1:A:163:LYS:HD2	2.03	0.40
1:A:179:ALA:HA	1:A:205:PRO:O	2.22	0.40
1:B:177:GLU:H	1:B:204:HIS:CE1	2.40	0.40
1:B:188:LEU:HB3	1:B:189:HIS:H	1.67	0.40
1:D:130:LEU:HD12	1:D:130:LEU:HA	1.95	0.40
1:C:177:GLU:H	1:C:204:HIS:CE1	2.40	0.40
1:D:54:ARG:NH1	1:D:79:LEU:HD21	2.37	0.40
1:F:91:ALA:HB1	1:F:126:ARG:CZ	2.52	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	227/286 (79%)	216 (95%)	11 (5%)	0	100	100
1	B	232/286 (81%)	225 (97%)	6 (3%)	1 (0%)	30	65
1	C	227/286 (79%)	218 (96%)	8 (4%)	1 (0%)	30	65
1	D	226/286 (79%)	218 (96%)	6 (3%)	2 (1%)	14	48
1	E	233/286 (82%)	221 (95%)	11 (5%)	1 (0%)	30	65
1	F	226/286 (79%)	212 (94%)	14 (6%)	0	100	100
All	All	1371/1716 (80%)	1310 (96%)	56 (4%)	5 (0%)	30	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	170	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	170	ALA
1	D	170	ALA
1	C	222	ASN
1	D	222	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	182/226 (80%)	180 (99%)	2 (1%)	65	83
1	B	185/226 (82%)	184 (100%)	1 (0%)	81	89
1	C	183/226 (81%)	180 (98%)	3 (2%)	55	79
1	D	182/226 (80%)	177 (97%)	5 (3%)	39	71
1	E	185/226 (82%)	184 (100%)	1 (0%)	81	89
1	F	181/226 (80%)	177 (98%)	4 (2%)	45	74
All	All	1098/1356 (81%)	1082 (98%)	16 (2%)	57	80

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	ASP
1	A	255	VAL
1	B	196	THR
1	C	186	SER
1	C	196	THR
1	C	203	ARG
1	D	72	THR
1	D	107	VAL
1	D	202	ASP
1	D	203	ARG
1	D	237	VAL
1	E	171	THR
1	F	196	THR
1	F	202	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	248	VAL
1	F	255	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	HIS
1	B	184	ASN
1	B	190	HIS
1	C	190	HIS
1	D	184	ASN
1	D	189	HIS
1	D	190	HIS
1	D	250	ASN
1	E	184	ASN
1	E	189	HIS
1	E	190	HIS
1	F	189	HIS
1	F	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 oligosaccharides 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	D	500	-	47,50,50	2.03	11 (23%)	69,75,75	1.67	11 (15%)
2	COA	F	600	-	47,50,50	2.02	11 (23%)	69,75,75	1.69	12 (17%)
2	COA	A	300	-	47,50,50	2.05	11 (23%)	69,75,75	1.69	12 (17%)
2	COA	E	400	-	47,50,50	2.04	11 (23%)	69,75,75	1.70	12 (17%)
2	COA	C	700	-	47,50,50	2.03	12 (25%)	69,75,75	1.66	11 (15%)

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	D	500	-	-	8/48/64/64	0/3/3/3
2	COA	F	600	-	-	12/48/64/64	0/3/3/3
2	COA	A	300	-	-	17/48/64/64	0/3/3/3
2	COA	E	400	-	-	7/48/64/64	0/3/3/3
2	COA	C	700	-	-	11/48/64/64	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	COA	C9P-N8P	6.13	1.48	1.33
2	E	400	COA	C9P-N8P	5.97	1.47	1.33
2	D	500	COA	C9P-N8P	5.89	1.47	1.33
2	C	700	COA	C9P-N8P	5.89	1.47	1.33
2	D	500	COA	C5P-N4P	5.81	1.47	1.33
2	A	300	COA	C5P-N4P	5.78	1.47	1.33
2	F	600	COA	C9P-N8P	5.63	1.46	1.33
2	E	400	COA	C5P-N4P	5.63	1.46	1.33
2	F	600	COA	C5P-N4P	5.53	1.46	1.33
2	C	700	COA	C5P-N4P	5.45	1.46	1.33
2	A	300	COA	C6A-N6A	4.64	1.46	1.34
2	F	600	COA	C6A-N6A	4.49	1.45	1.34
2	D	500	COA	C6A-N6A	4.45	1.45	1.34
2	E	400	COA	C6A-N6A	4.43	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	600	COA	C2B-C3B	-4.34	1.43	1.53
2	E	400	COA	C2B-C3B	-4.34	1.43	1.53
2	D	500	COA	C2B-C3B	-4.31	1.43	1.53
2	A	300	COA	C2B-C3B	-4.28	1.43	1.53
2	C	700	COA	C6A-N6A	4.28	1.45	1.34
2	C	700	COA	C2B-C3B	-4.24	1.43	1.53
2	C	700	COA	OAP-CAP	-3.86	1.35	1.42
2	A	300	COA	OAP-CAP	-3.67	1.35	1.42
2	E	400	COA	OAP-CAP	-3.66	1.35	1.42
2	F	600	COA	OAP-CAP	-3.66	1.35	1.42
2	E	400	COA	C2B-C1B	-3.48	1.42	1.53
2	F	600	COA	C2B-C1B	-3.46	1.42	1.53
2	D	500	COA	OAP-CAP	-3.43	1.36	1.42
2	D	500	COA	C2B-C1B	-3.43	1.42	1.53
2	C	700	COA	C2B-C1B	-3.36	1.42	1.53
2	C	700	COA	P1A-O3A	-3.34	1.55	1.59
2	A	300	COA	C2B-C1B	-3.20	1.43	1.53
2	E	400	COA	C1B-N9A	-3.20	1.37	1.46
2	F	600	COA	P1A-O3A	-3.18	1.56	1.59
2	F	600	COA	C3B-C4B	-3.07	1.45	1.52
2	F	600	COA	C1B-N9A	-3.05	1.37	1.46
2	D	500	COA	C3B-C4B	-3.02	1.45	1.52
2	D	500	COA	C1B-N9A	-2.98	1.38	1.46
2	A	300	COA	C3B-C4B	-2.97	1.45	1.52
2	C	700	COA	C1B-N9A	-2.90	1.38	1.46
2	E	400	COA	P1A-O3A	-2.89	1.56	1.59
2	E	400	COA	C3B-C4B	-2.87	1.45	1.52
2	C	700	COA	C3B-C4B	-2.85	1.45	1.52
2	D	500	COA	P1A-O3A	-2.77	1.56	1.59
2	A	300	COA	O4B-C1B	2.76	1.48	1.42
2	C	700	COA	O4B-C1B	2.73	1.48	1.42
2	A	300	COA	P1A-O3A	-2.70	1.56	1.59
2	A	300	COA	C1B-N9A	-2.68	1.38	1.46
2	D	500	COA	O4B-C1B	2.68	1.48	1.42
2	E	400	COA	O4B-C1B	2.58	1.48	1.42
2	F	600	COA	O4B-C1B	2.51	1.47	1.42
2	E	400	COA	C8A-N9A	-2.30	1.33	1.37
2	C	700	COA	C8A-N9A	-2.21	1.33	1.37
2	A	300	COA	C8A-N9A	-2.18	1.33	1.37
2	C	700	COA	C5A-N7A	-2.13	1.35	1.39
2	F	600	COA	C8A-N9A	-2.12	1.33	1.37
2	D	500	COA	C8A-N9A	-2.02	1.34	1.37

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	COA	C5A-C4A-N3A	-5.74	118.81	126.72
2	F	600	COA	N3A-C2A-N1A	-5.60	120.10	128.58
2	C	700	COA	C5A-C4A-N3A	-5.55	119.07	126.72
2	D	500	COA	N3A-C2A-N1A	-5.53	120.21	128.58
2	C	700	COA	N3A-C2A-N1A	-5.46	120.31	128.58
2	E	400	COA	N3A-C2A-N1A	-5.44	120.35	128.58
2	A	300	COA	N3A-C2A-N1A	-5.43	120.36	128.58
2	D	500	COA	C5A-C4A-N3A	-5.27	119.45	126.72
2	E	400	COA	C5A-C4A-N3A	-5.09	119.70	126.72
2	F	600	COA	C5A-C4A-N3A	-4.97	119.88	126.72
2	A	300	COA	N3A-C4A-N9A	4.68	135.13	127.17
2	C	700	COA	N3A-C4A-N9A	4.66	135.09	127.17
2	D	500	COA	N3A-C4A-N9A	4.47	134.77	127.17
2	E	400	COA	N3A-C4A-N9A	4.35	134.56	127.17
2	F	600	COA	N3A-C4A-N9A	4.31	134.50	127.17
2	A	300	COA	C5A-N7A-C8A	3.82	109.46	103.45
2	C	700	COA	C5A-N7A-C8A	3.79	109.40	103.45
2	E	400	COA	C5A-N7A-C8A	3.74	109.33	103.45
2	A	300	COA	C2A-N3A-C4A	3.73	120.95	111.83
2	F	600	COA	C5A-N7A-C8A	3.73	109.31	103.45
2	D	500	COA	C5A-N7A-C8A	3.64	109.17	103.45
2	C	700	COA	C2A-N3A-C4A	3.63	120.70	111.83
2	D	500	COA	C2A-N3A-C4A	3.58	120.58	111.83
2	E	400	COA	C2A-N3A-C4A	3.48	120.32	111.83
2	F	600	COA	C2A-N3A-C4A	3.47	120.30	111.83
2	F	600	COA	N9A-C8A-N7A	-3.36	109.17	113.94
2	E	400	COA	N9A-C8A-N7A	-3.33	109.20	113.94
2	D	500	COA	C6P-C7P-N8P	-3.23	105.13	112.00
2	D	500	COA	N9A-C8A-N7A	-3.18	109.42	113.94
2	C	700	COA	N9A-C8A-N7A	-3.13	109.50	113.94
2	A	300	COA	C4A-C5A-N7A	-3.02	107.12	110.58
2	A	300	COA	N9A-C8A-N7A	-2.89	109.84	113.94
2	E	400	COA	C4A-C5A-N7A	-2.87	107.30	110.58
2	C	700	COA	C4A-C5A-N7A	-2.77	107.41	110.58
2	F	600	COA	C4A-C5A-N7A	-2.71	107.48	110.58
2	D	500	COA	O6A-CCP-CBP	2.70	114.89	110.55
2	D	500	COA	C4A-C5A-N7A	-2.68	107.52	110.58
2	E	400	COA	C4A-N9A-C8A	2.56	108.43	105.74
2	F	600	COA	CAP-C9P-N8P	2.56	121.33	116.48
2	F	600	COA	C4A-N9A-C8A	2.54	108.41	105.74
2	E	400	COA	CAP-C9P-N8P	2.53	121.28	116.48
2	E	400	COA	CEP-CBP-CAP	2.53	113.08	108.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	COA	CEP-CBP-CAP	2.43	112.90	108.77
2	F	600	COA	C7P-N8P-C9P	-2.36	118.30	122.55
2	A	300	COA	C2P-C3P-N4P	-2.35	106.97	112.31
2	D	500	COA	C4A-N9A-C8A	2.27	108.13	105.74
2	F	600	COA	C6P-C5P-N4P	2.26	120.46	116.34
2	C	700	COA	CAP-C9P-N8P	2.24	120.74	116.48
2	E	400	COA	C6P-C7P-N8P	-2.23	107.25	112.00
2	D	500	COA	C4B-O4B-C1B	-2.23	104.54	109.47
2	E	400	COA	C4B-O4B-C1B	-2.17	104.68	109.47
2	C	700	COA	C4B-O4B-C1B	-2.14	104.74	109.47
2	F	600	COA	C4B-O4B-C1B	-2.14	104.75	109.47
2	A	300	COA	C3B-C2B-C1B	2.11	104.53	99.89
2	A	300	COA	C4B-O4B-C1B	-2.10	104.83	109.47
2	C	700	COA	C6P-C7P-N8P	-2.10	107.53	112.00
2	A	300	COA	CAP-C9P-N8P	2.01	120.30	116.48
2	C	700	COA	C4A-N9A-C8A	2.00	107.84	105.74

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	COA	C4B-C3B-O3B-P3B
2	A	300	COA	O4B-C4B-C5B-O5B
2	A	300	COA	C5B-O5B-P1A-O3A
2	A	300	COA	C5P-C6P-C7P-N8P
2	C	700	COA	C5B-O5B-P1A-O1A
2	C	700	COA	C5B-O5B-P1A-O2A
2	C	700	COA	S1P-C2P-C3P-N4P
2	D	500	COA	O4B-C4B-C5B-O5B
2	D	500	COA	C5B-O5B-P1A-O1A
2	D	500	COA	C5B-O5B-P1A-O3A
2	D	500	COA	O9P-C9P-CAP-OAP
2	E	400	COA	S1P-C2P-C3P-N4P
2	F	600	COA	CCP-O6A-P2A-O5A
2	F	600	COA	CDP-CBP-CCP-O6A
2	F	600	COA	CEP-CBP-CCP-O6A
2	F	600	COA	CAP-CBP-CCP-O6A
2	F	600	COA	O9P-C9P-CAP-CBP
2	F	600	COA	N8P-C9P-CAP-CBP
2	A	300	COA	C3B-C4B-C5B-O5B
2	D	500	COA	C3B-C4B-C5B-O5B
2	C	700	COA	C3B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	700	COA	O4B-C4B-C5B-O5B
2	A	300	COA	C2B-C3B-O3B-P3B
2	C	700	COA	O9P-C9P-CAP-OAP
2	F	600	COA	N8P-C9P-CAP-OAP
2	D	500	COA	C5P-C6P-C7P-N8P
2	A	300	COA	P1A-O3A-P2A-O4A
2	A	300	COA	CDP-CBP-CCP-O6A
2	A	300	COA	CEP-CBP-CCP-O6A
2	E	400	COA	CDP-CBP-CCP-O6A
2	E	400	COA	CEP-CBP-CCP-O6A
2	C	700	COA	C2B-C1B-N9A-C8A
2	D	500	COA	C2P-C3P-N4P-C5P
2	A	300	COA	C5B-O5B-P1A-O1A
2	A	300	COA	CCP-O6A-P2A-O4A
2	C	700	COA	C5B-O5B-P1A-O3A
2	F	600	COA	CCP-O6A-P2A-O3A
2	F	600	COA	CCP-O6A-P2A-O4A
2	E	400	COA	C5P-C6P-C7P-N8P
2	E	400	COA	C3B-O3B-P3B-O9A
2	A	300	COA	C2P-C3P-N4P-C5P
2	D	500	COA	N8P-C9P-CAP-OAP
2	A	300	COA	C3B-O3B-P3B-O7A
2	F	600	COA	C4B-C3B-O3B-P3B
2	C	700	COA	P1A-O3A-P2A-O4A
2	F	600	COA	C3B-O3B-P3B-O8A
2	A	300	COA	O9P-C9P-CAP-OAP
2	C	700	COA	O4B-C1B-N9A-C8A
2	F	600	COA	C5P-C6P-C7P-N8P
2	E	400	COA	C4B-C3B-O3B-P3B
2	A	300	COA	N8P-C9P-CAP-OAP
2	C	700	COA	N8P-C9P-CAP-OAP
2	E	400	COA	N8P-C9P-CAP-OAP
2	A	300	COA	CAP-CBP-CCP-O6A
2	A	300	COA	P1A-O3A-P2A-O5A

There are no ring outliers.

5 monomers are involved in 9 short contacts:

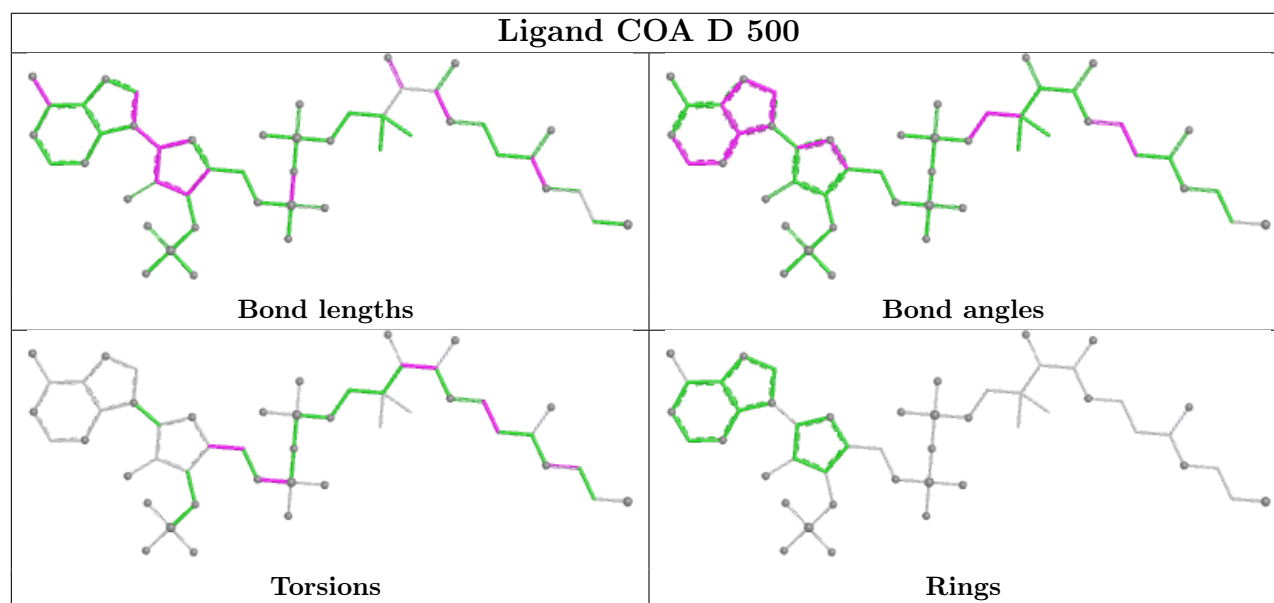
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	COA	1	0
2	F	600	COA	1	0
2	A	300	COA	3	0

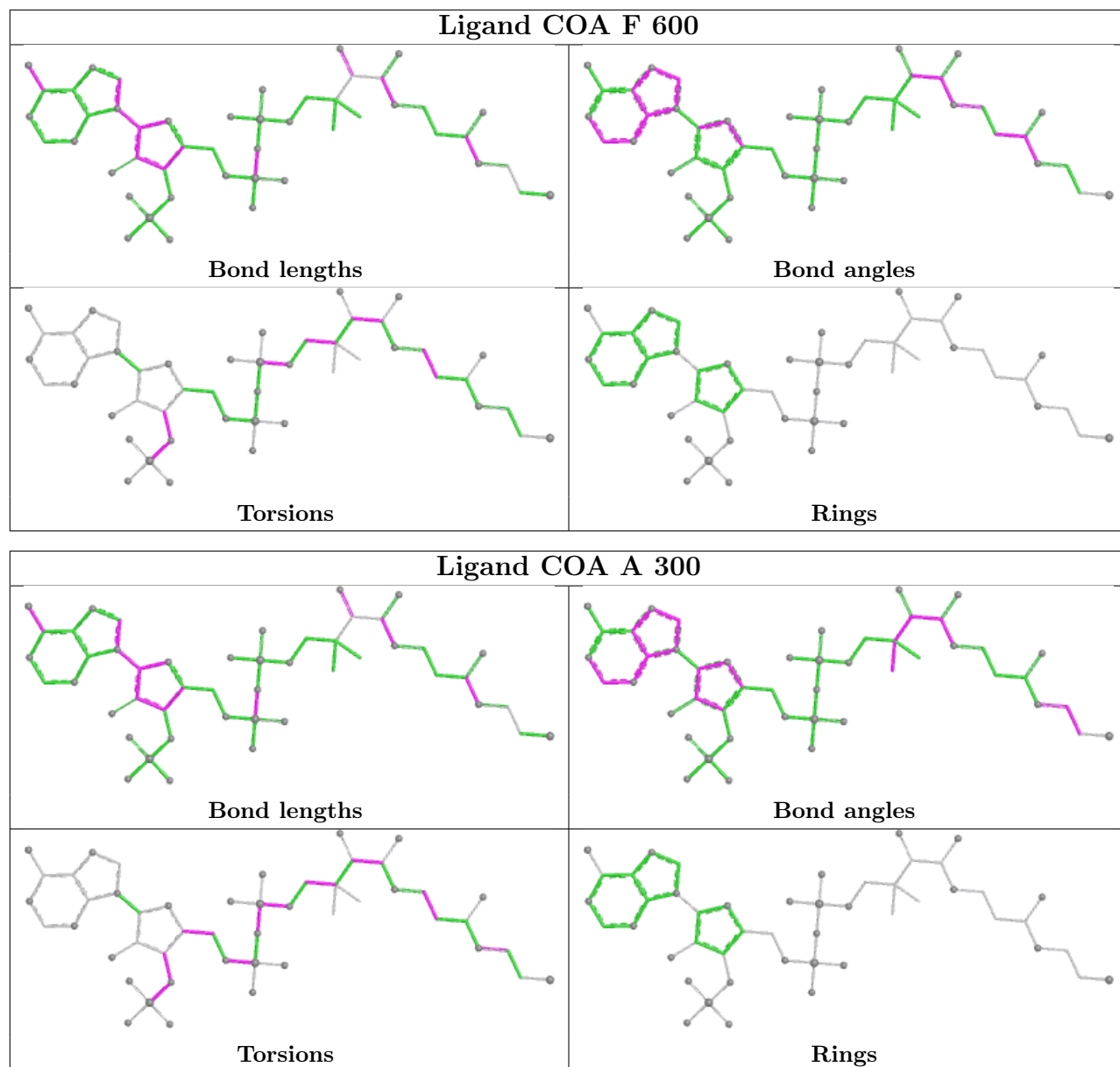
Continued on next page...

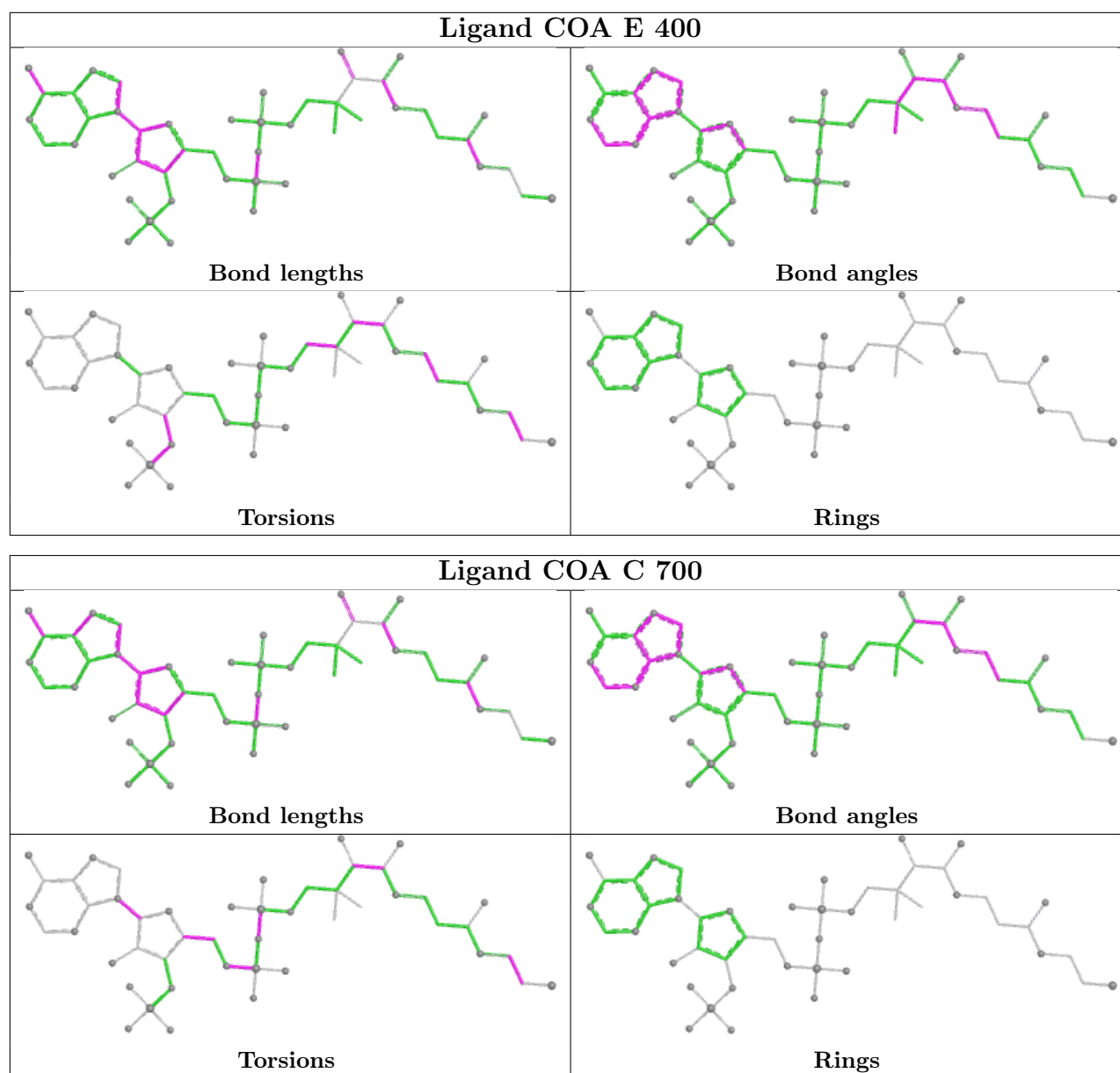
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	400	COA	3	0
2	C	700	COA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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, 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%)	-0.42	4 (1%)	69 45	31, 54, 89, 153	0
1	B	236/286 (82%)	-0.34	4 (1%)	69 45	34, 67, 110, 187	0
1	C	233/286 (81%)	-0.37	1 (0%)	88 76	33, 62, 93, 113	0
1	D	232/286 (81%)	-0.41	5 (2%)	62 39	34, 64, 94, 133	0
1	E	237/286 (82%)	-0.40	2 (0%)	82 64	34, 64, 103, 154	0
1	F	232/286 (81%)	-0.46	2 (0%)	81 61	36, 69, 100, 120	0
All	All	1403/1716 (81%)	-0.40	18 (1%)	75 53	31, 64, 99, 187	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	107	VAL	4.1
1	D	103	ASP	3.0
1	B	168	ASP	2.9
1	C	189	HIS	2.8
1	A	171	THR	2.8
1	A	189	HIS	2.8
1	B	197	GLY	2.8
1	D	19	TRP	2.7
1	B	104	PRO	2.6
1	B	111	HIS	2.6
1	D	170	ALA	2.5
1	F	103	ASP	2.5
1	E	199	VAL	2.4
1	E	104	PRO	2.4
1	A	31	ASP	2.1
1	A	107	VAL	2.0
1	F	239	ILE	2.0
1	D	109	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

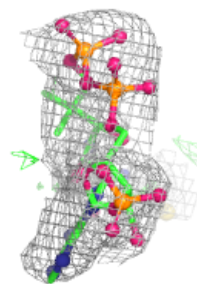
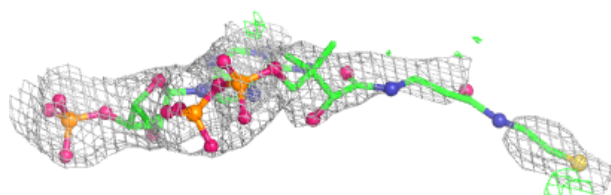
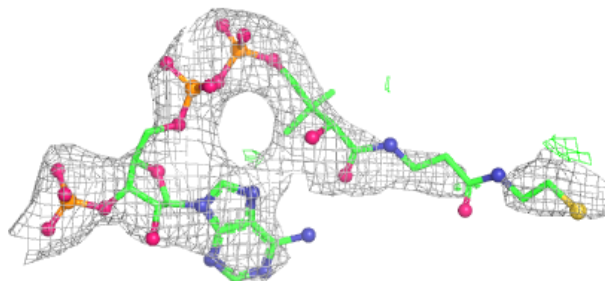
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	COA	D	500	48/48	0.78	0.11	62,129,158,283	0
2	COA	A	300	48/48	0.85	0.13	67,105,128,226	48
2	COA	E	400	48/48	0.88	0.10	52,94,125,233	0
2	COA	C	700	48/48	0.91	0.09	53,94,117,171	0
2	COA	F	600	48/48	0.92	0.08	61,92,132,198	0

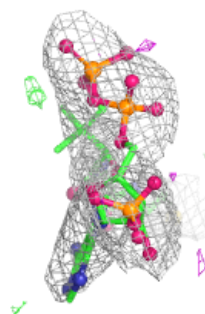
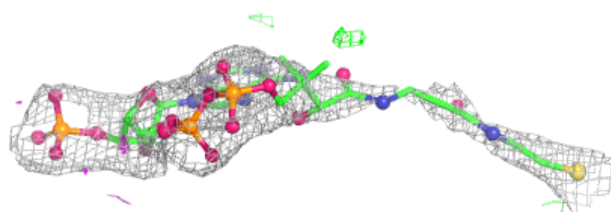
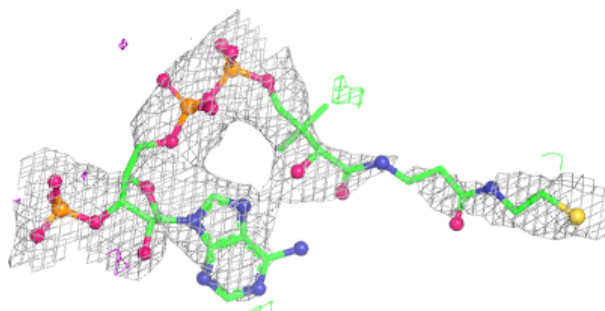
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA D 500:

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

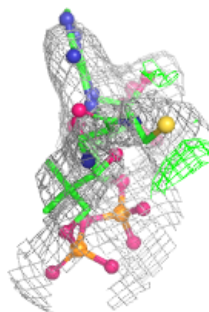
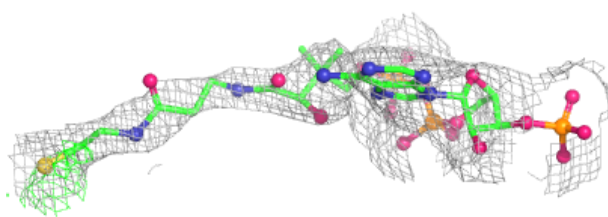
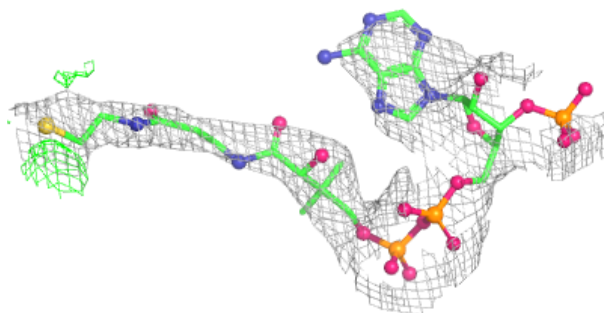
**Electron density around COA A 300:**

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

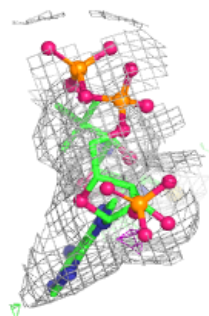
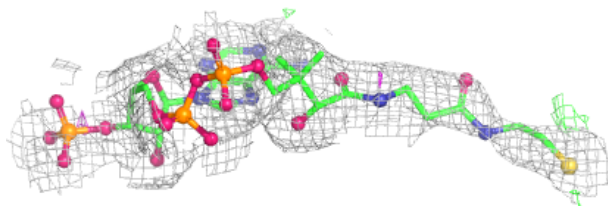
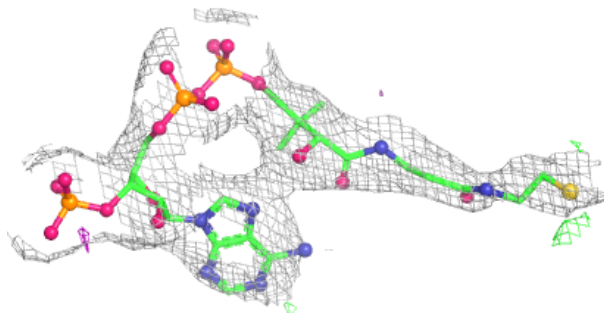


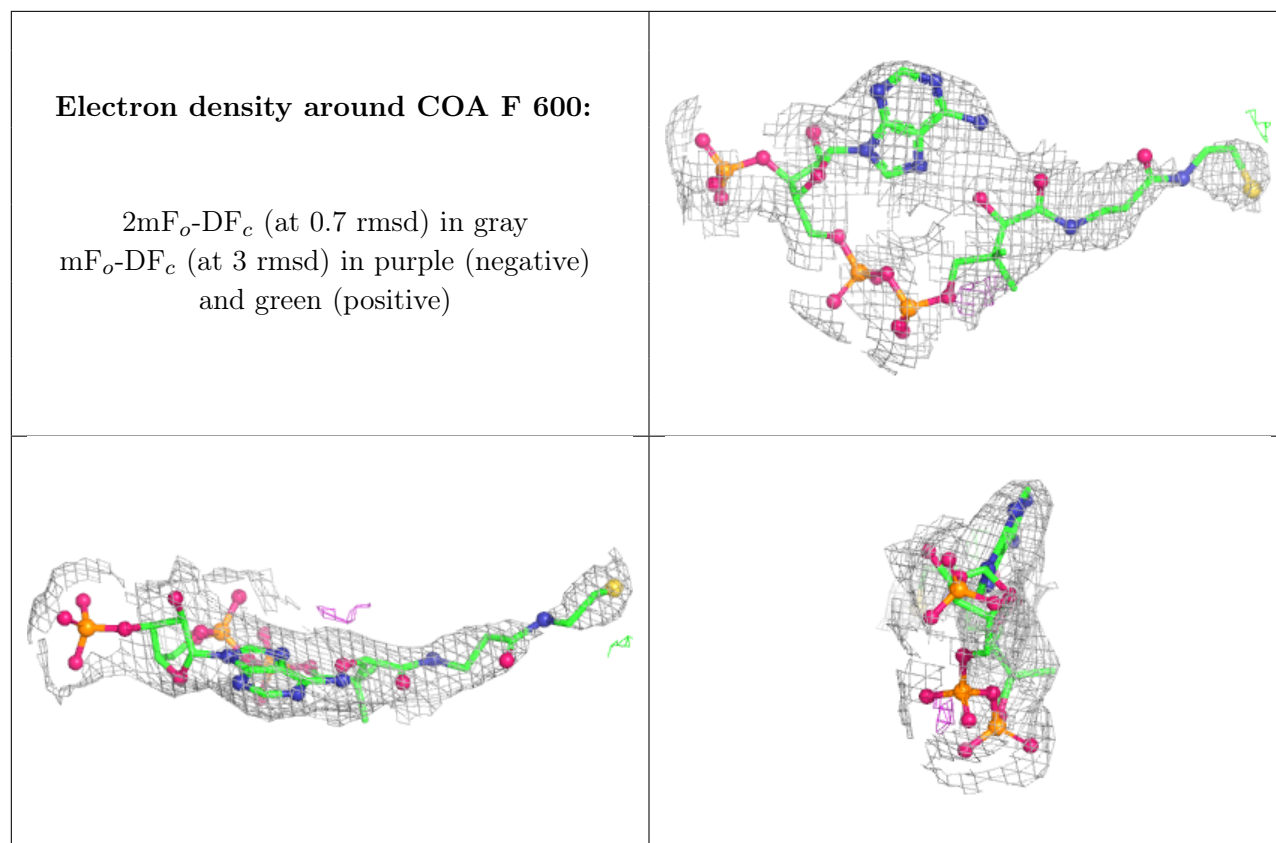
Electron density around COA E 400:

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

**Electron density around COA C 700:**

$2mF_o-DF_c$ (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.