Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 01:43 AM BST

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

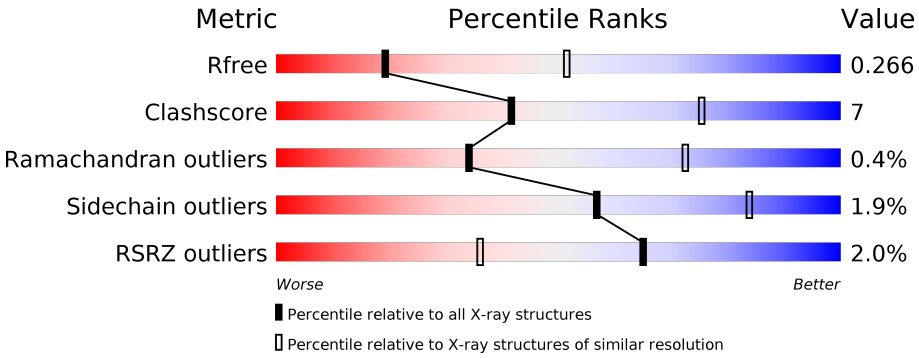
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	286	66% 14% • 19%
1	B	286	69% 13% • 17%
1	C	286	64% 16% • 19%
1	D	286	62% 19% 19%
1	E	286	71% 11% 17%
1	F	286	68% 12% • 19%

2 Entry composition (i)

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

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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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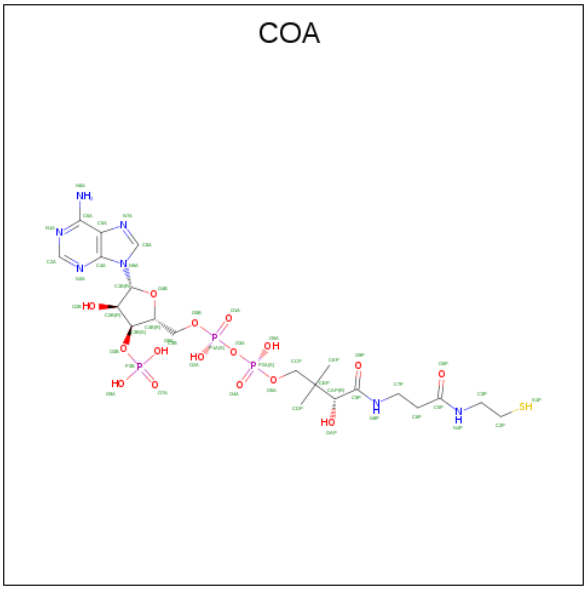
Chain	Residue	Modelled	Actual	Comment	Reference
E	53	GLU	VAL	SEE REMARK 999	UNP I1KHY6
E	84	SER	PHE	SEE REMARK 999	UNP I1KHY6
E	89	ARG	CYS	SEE REMARK 999	UNP I1KHY6
E	137	ARG	GLN	SEE REMARK 999	UNP I1KHY6
E	149	ASN	ASP	SEE REMARK 999	UNP I1KHY6
E	244	ARG	GLN	SEE REMARK 999	UNP I1KHY6
F	7	ALA	LYS	SEE 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: $C_{21}H_{36}N_7O_{16}P_3S$).



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		

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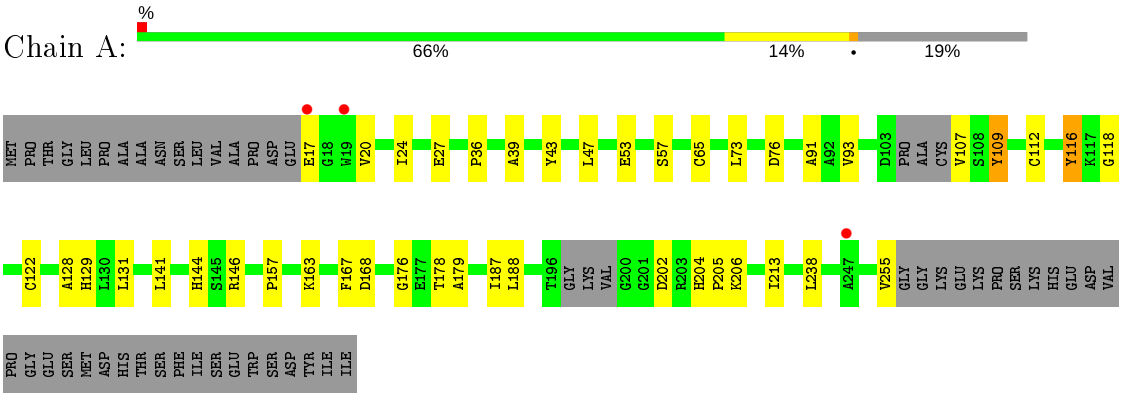
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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.

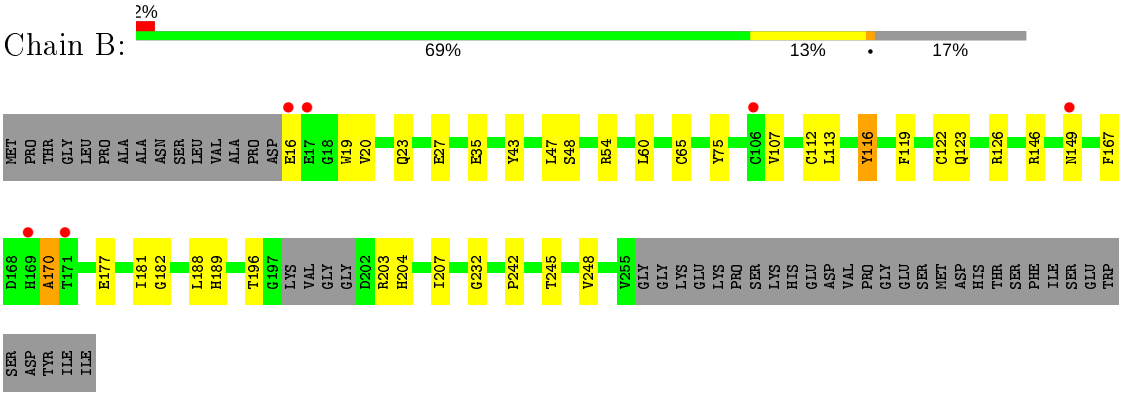
- Molecule 1: Serine Acetyltransferase Apoenzyme

Chain A:



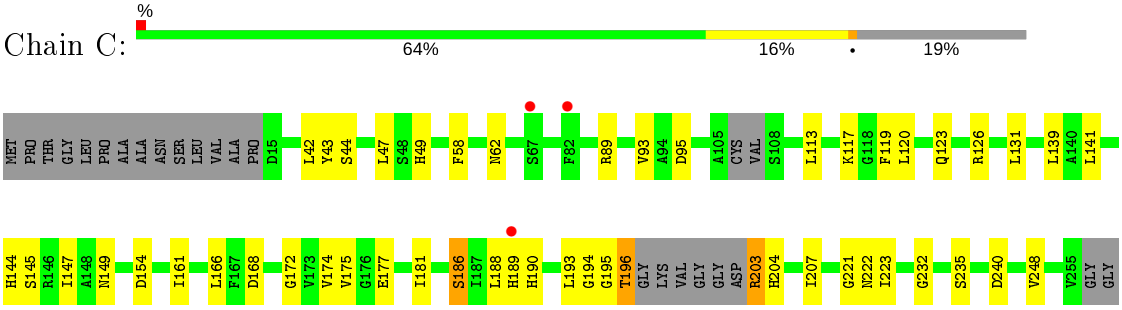
- Molecule 1: Serine Acetyltransferase Apoenzyme

Chain B:



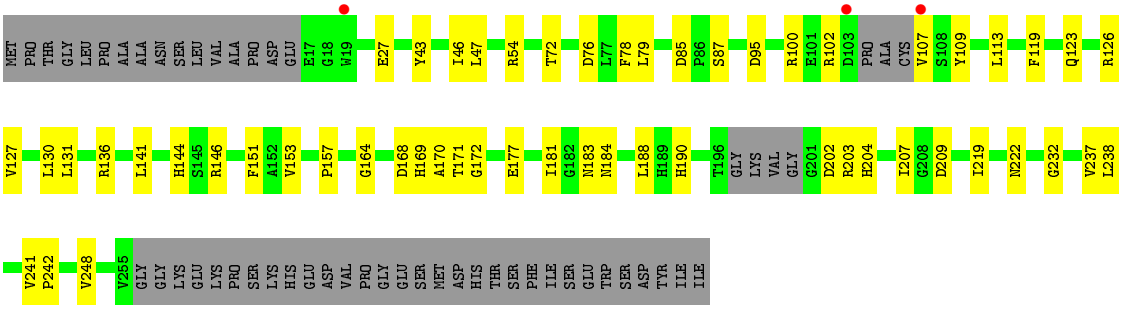
- Molecule 1: Serine Acetyltransferase Apoenzyme

Chain C:



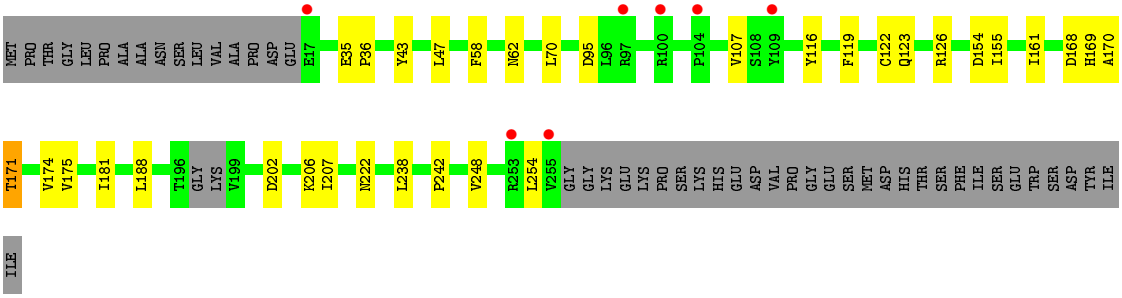
• Molecule 1: Serine Acetyltransferase Apoenzyme

Chain D:



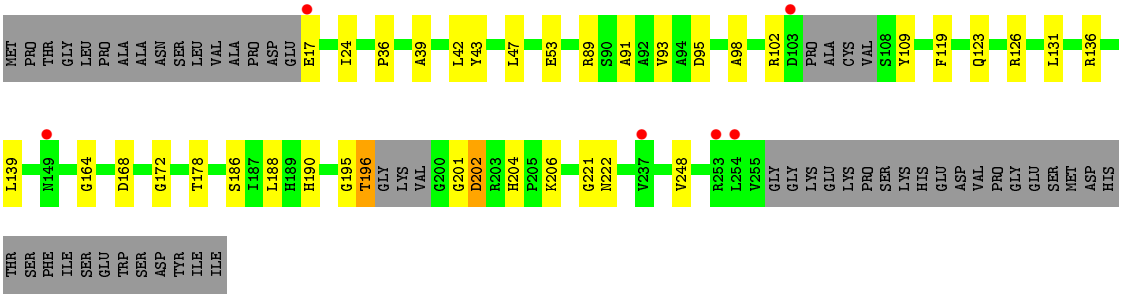
• Molecule 1: Serine Acetyltransferase Apoenzyme

Chain E:



• Molecule 1: Serine Acetyltransferase Apoenzyme

Chain F:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	0.69 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.214 , 0.268 0.217 , 0.266	Depositor DCC
R_{free} test set	2000 reflections (4.67%)	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)	0.28 , 22.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.49	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

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.

All (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
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:F:204:HIS:O	1:F:206:LYS:NZ	2.32	0.62
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: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
1:A:65:CYS:O	1:A:146:ARG:NH2	2.35	0.57
1:F:196:THR:OG1	1:F:196:THR:O	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:H8A	2:A:300:COA:O5B	2.07	0.55
1:E:161:ILE:HG22	1:E:181:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:232:GLY:O	1:C:235:SER:OG	2.22	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HD11	2:D:500:COA:C5A	2.45	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:167:PHE:HB3	1:B:170:ALA:HB2	1.99	0.44
1:B:19:TRP:CZ3	1:B:23:GLN:HG3	2.53	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:N7A	2:A:300:COA:H133	2.33	0.43
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:C:42:LEU:HD23	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:43:TYR:HA	1:A:47:LEU:HB2	2.01	0.42
1:A:17:GLU:HB2	1:A:93:VAL:HG21	2.01	0.42
2:C:700:COA:H2B	2:C:700:COA:H8A	1.84	0.42
1:F:53:GLU:OE2	1:F:89:ARG:HD2	2.18	0.42
2:E:400:COA:N7A	2:E:400:COA:H133	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:HA	1:B:60:LEU:HD23	1.88	0.41
1:F:42:LEU:HA	1:F:42:LEU:HD23	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:HD2	1:A:146:ARG:HA	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:141:LEU:HA	1:D:141:LEU:HD23	1.90	0.41
1:D:95:ASP:OD2	1:D:123:GLN:NE2	2.52	0.41
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:179:ALA:HA	1:A:205:PRO:O	2.22	0.40
1:A:91:ALA:HA	1:A:163:LYS:HD2	2.03	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:HA	1:D:130:LEU:HD12	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%)	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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	TYR
1	A	116	TYR
1	A	202	ASP
1	A	255	VAL
1	B	75	TYR
1	B	116	TYR
1	B	196	THR
1	B	203	ARG
1	C	186	SER
1	C	196	THR
1	C	203	ARG
1	D	72	THR
1	D	107	VAL
1	D	144	HIS
1	D	202	ASP
1	D	203	ARG
1	E	171	THR
1	E	202	ASP
1	F	196	THR
1	F	202	ASP
1	F	248	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	HIS
1	C	190	HIS
1	D	189	HIS
1	D	190	HIS

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	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%)
2	COA	D	500	-	41,50,50	2.35	8 (19%)	52,75,75	1.32	4 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	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	F	600	-	-	11/44/64/64	0/3/3/3
2	COA	A	300	-	-	13/44/64/64	0/3/3/3
2	COA	D	500	-	-	8/44/64/64	0/3/3/3

All (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
2	A	300	COA	C9P-N8P	6.58	1.48	1.33
2	E	400	COA	C9P-N8P	6.42	1.47	1.33
2	D	500	COA	C9P-N8P	6.33	1.47	1.33
2	C	700	COA	C9P-N8P	6.32	1.47	1.33
2	D	500	COA	C5P-N4P	6.06	1.47	1.33
2	F	600	COA	C9P-N8P	6.04	1.46	1.33
2	A	300	COA	C5P-N4P	6.03	1.47	1.33
2	E	400	COA	C5P-N4P	5.87	1.46	1.33
2	F	600	COA	C5P-N4P	5.77	1.46	1.33
2	C	700	COA	C5P-N4P	5.69	1.46	1.33
2	A	300	COA	O4B-C1B	5.24	1.48	1.41
2	C	700	COA	O4B-C1B	5.19	1.48	1.41
2	D	500	COA	O4B-C1B	5.10	1.48	1.41
2	E	400	COA	O4B-C1B	4.94	1.48	1.41
2	F	600	COA	O4B-C1B	4.81	1.47	1.41
2	F	600	COA	C2B-C3B	-4.24	1.43	1.52
2	E	400	COA	C2B-C3B	-4.24	1.43	1.52
2	D	500	COA	C2B-C3B	-4.21	1.43	1.52
2	A	300	COA	C2B-C3B	-4.18	1.43	1.52
2	C	700	COA	C2B-C3B	-4.14	1.43	1.52
2	C	700	COA	OAP-CAP	-3.70	1.35	1.42
2	A	300	COA	OAP-CAP	-3.52	1.35	1.42
2	E	400	COA	OAP-CAP	-3.52	1.35	1.42
2	F	600	COA	OAP-CAP	-3.51	1.35	1.42
2	D	500	COA	OAP-CAP	-3.29	1.36	1.42
2	A	300	COA	C6A-N6A	3.29	1.46	1.34
2	F	600	COA	C6A-N6A	3.19	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	COA	C6A-N6A	3.16	1.45	1.34
2	E	400	COA	C6A-N6A	3.14	1.45	1.34
2	C	700	COA	C6A-N6A	3.04	1.45	1.34
2	F	600	COA	C3B-C4B	-2.94	1.45	1.52
2	D	500	COA	C3B-C4B	-2.89	1.45	1.52
2	A	300	COA	C3B-C4B	-2.85	1.45	1.52
2	E	400	COA	C3B-C4B	-2.75	1.45	1.52
2	C	700	COA	C3B-C4B	-2.73	1.45	1.52
2	C	700	COA	C2A-N3A	2.13	1.35	1.32

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
2	F	600	COA	P2A-O3A-P1A	-4.29	118.11	132.83
2	E	400	COA	P2A-O3A-P1A	-4.27	118.17	132.83
2	C	700	COA	P2A-O3A-P1A	-4.26	118.22	132.83
2	A	300	COA	P2A-O3A-P1A	-3.61	120.43	132.83
2	D	500	COA	C6P-C7P-N8P	-3.35	105.13	111.90
2	D	500	COA	P2A-O3A-P1A	-3.05	122.35	132.83
2	D	500	COA	O6A-CCP-CBP	2.70	114.89	110.55
2	E	400	COA	CEP-CBP-CAP	2.46	113.08	108.82
2	F	600	COA	C7P-N8P-C9P	-2.41	118.30	122.59
2	F	600	COA	C6P-C5P-N4P	2.40	120.46	116.42
2	F	600	COA	CAP-C9P-N8P	2.39	121.33	116.58
2	E	400	COA	CAP-C9P-N8P	2.36	121.28	116.58
2	A	300	COA	CEP-CBP-CAP	2.35	112.90	108.82
2	A	300	COA	C2P-C3P-N4P	-2.34	106.97	112.31
2	E	400	COA	C6P-C7P-N8P	-2.30	107.25	111.90
2	A	300	COA	C4A-C5A-N7A	-2.18	107.12	109.40
2	C	700	COA	C6P-C7P-N8P	-2.16	107.53	111.90
2	A	300	COA	C3B-C2B-C1B	2.09	104.53	99.89
2	C	700	COA	CAP-C9P-N8P	2.09	120.74	116.58
2	E	400	COA	C6P-C5P-N4P	2.03	119.84	116.42
2	E	400	COA	C4A-C5A-N7A	-2.01	107.30	109.40

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	700	COA	C5B-O5B-P1A-O1A
2	C	700	COA	C5B-O5B-P1A-O2A
2	C	700	COA	C5B-O5B-P1A-O3A
2	C	700	COA	S1P-C2P-C3P-N4P
2	E	400	COA	C3B-O3B-P3B-O9A
2	E	400	COA	S1P-C2P-C3P-N4P
2	D	500	COA	C3B-C4B-C5B-O5B
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	F	600	COA	CCP-O6A-P2A-O3A
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	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
2	C	700	COA	C3B-C4B-C5B-O5B
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	F	600	COA	CCP-O6A-P2A-O4A
2	A	300	COA	C5B-O5B-P1A-O1A
2	D	500	COA	C2P-C3P-N4P-C5P
2	E	400	COA	CEP-CBP-CCP-O6A
2	A	300	COA	CEP-CBP-CCP-O6A
2	E	400	COA	C5P-C6P-C7P-N8P
2	A	300	COA	C2P-C3P-N4P-C5P
2	E	400	COA	CDP-CBP-CCP-O6A
2	A	300	COA	CDP-CBP-CCP-O6A
2	D	500	COA	N8P-C9P-CAP-OAP
2	F	600	COA	C4B-C3B-O3B-P3B
2	F	600	COA	C3B-O3B-P3B-O9A
2	A	300	COA	C3B-O3B-P3B-O9A

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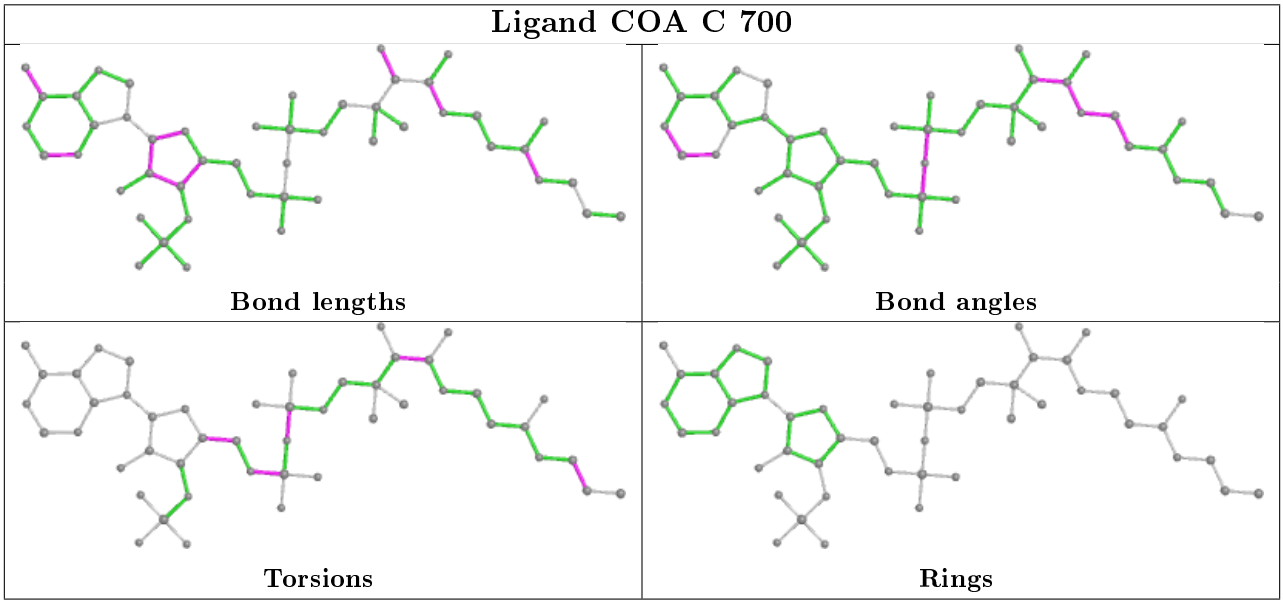
Mol	Chain	Res	Type	Atoms
2	C	700	COA	P1A-O3A-P2A-O4A
2	A	300	COA	CCP-O6A-P2A-O4A
2	E	400	COA	C4B-C3B-O3B-P3B

There are no ring outliers.

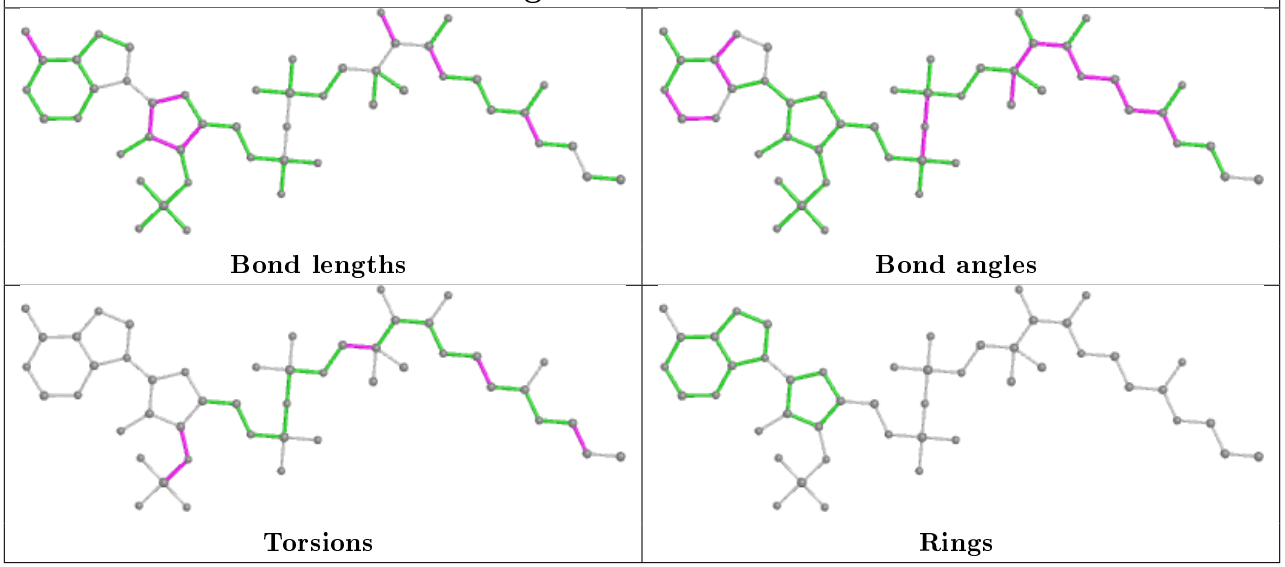
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	700	COA	1	0
2	E	400	COA	3	0
2	F	600	COA	1	0
2	A	300	COA	3	0
2	D	500	COA	1	0

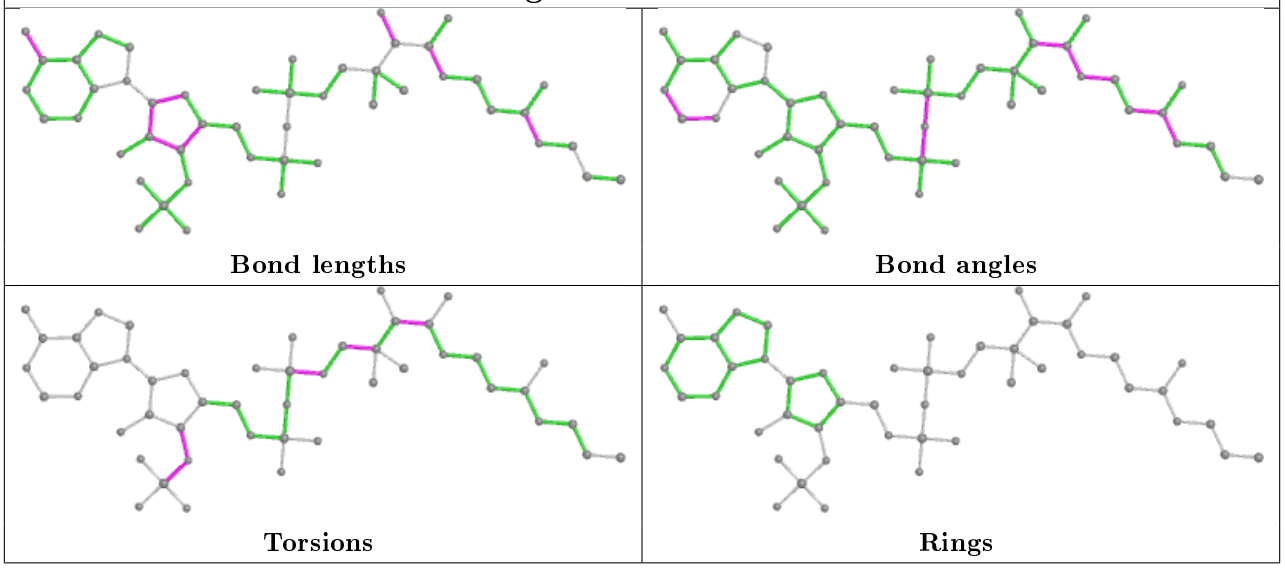
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

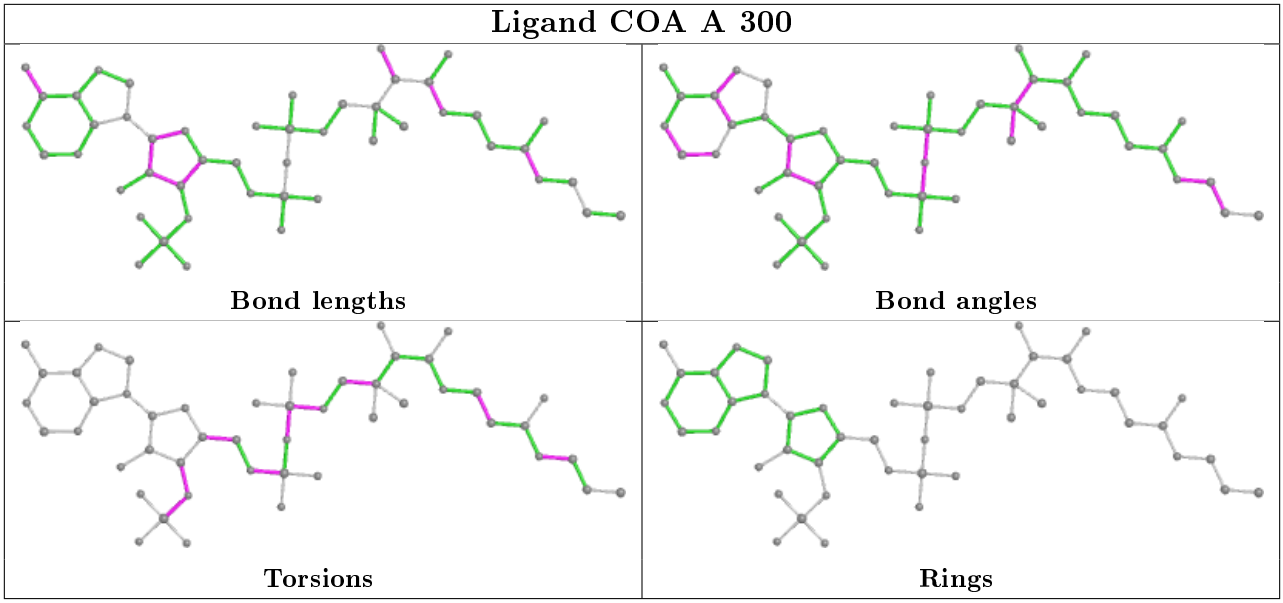


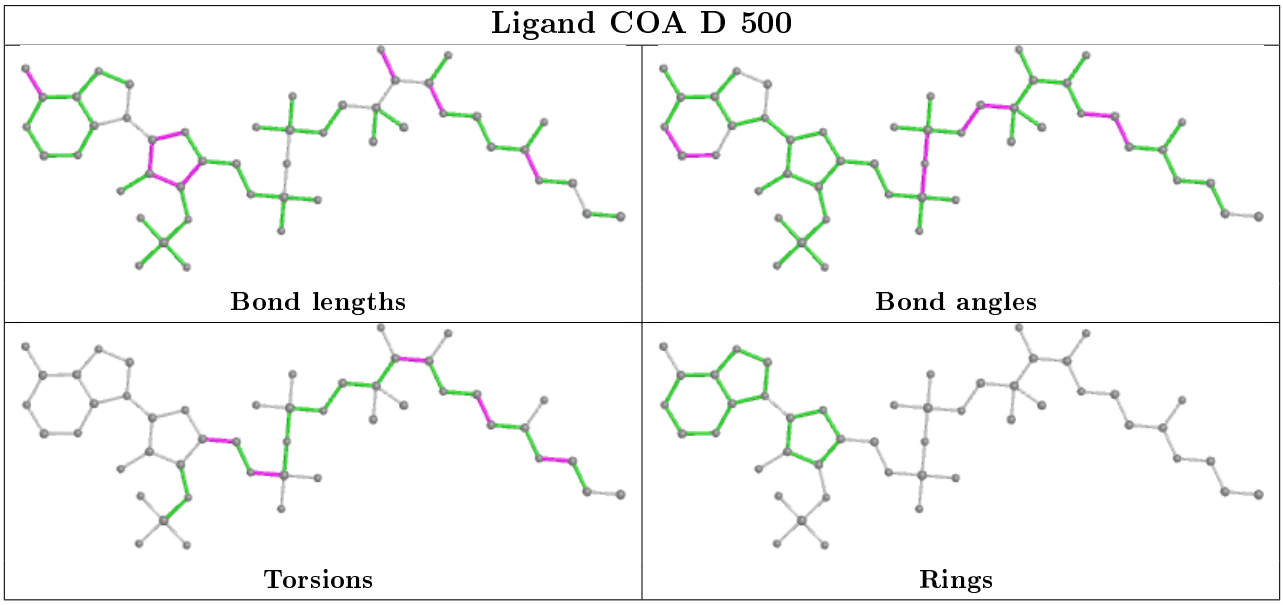
Ligand COA E 400



Ligand COA F 600







5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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

All (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
1	D	103	ASP	2.9
1	E	253	ARG	2.9
1	E	100	ARG	2.8
1	F	254	LEU	2.7
1	B	149	ASN	2.5
1	F	149	ASN	2.5
1	D	107	VAL	2.4
1	A	17	GLU	2.3
1	E	97	ARG	2.3
1	A	247	ALA	2.3
1	F	103	ASP	2.3
1	B	16	GLU	2.2
1	E	17	GLU	2.2
1	C	67	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	189	HIS	2.2
1	A	19	TRP	2.1
1	C	82	PHE	2.1
1	E	255	VAL	2.1
1	F	237	VAL	2.1
1	F	253	ARG	2.1
1	B	17	GLU	2.0
1	B	171	THR	2.0
1	B	169	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

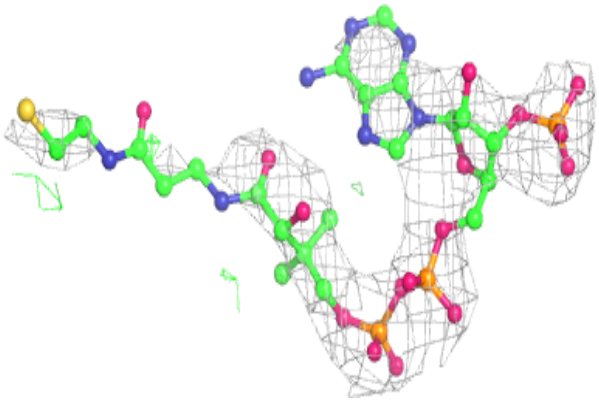
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

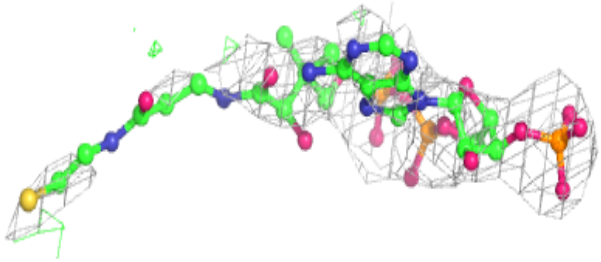
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	COA	D	500	48/48	0.80	0.44	62,129,158,283	0
2	COA	E	400	48/48	0.87	0.27	52,94,125,233	0
2	COA	A	300	48/48	0.88	0.33	67,105,128,226	48
2	COA	C	700	48/48	0.90	0.18	53,94,117,171	0
2	COA	F	600	48/48	0.92	0.16	61,92,132,198	0

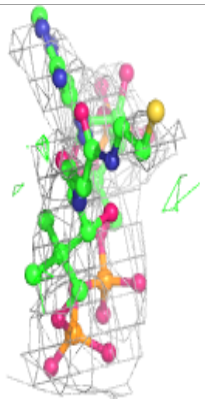
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

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)

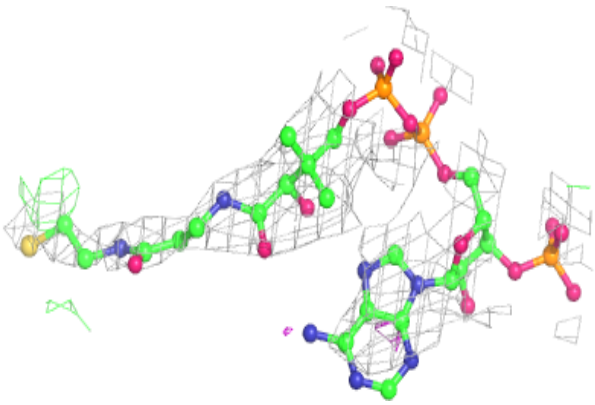


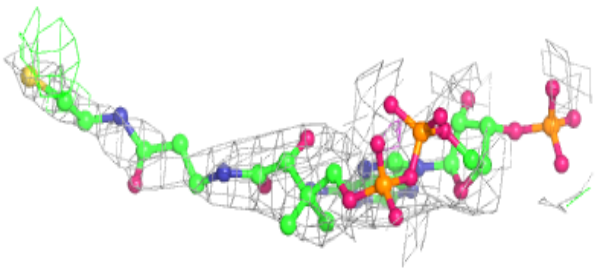


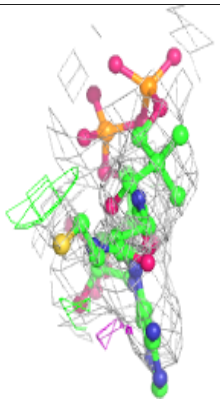


Electron density around COA E 400:

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

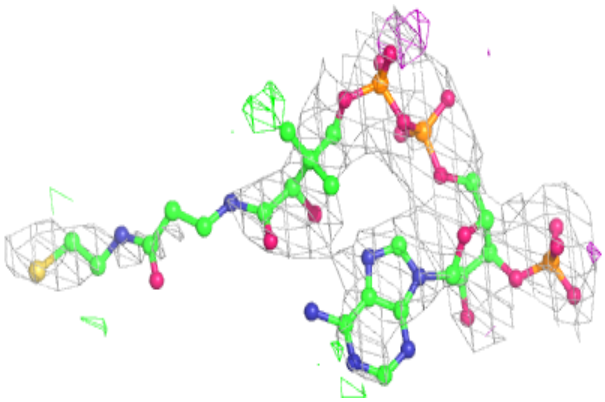


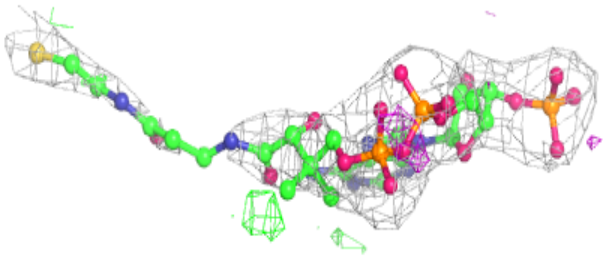


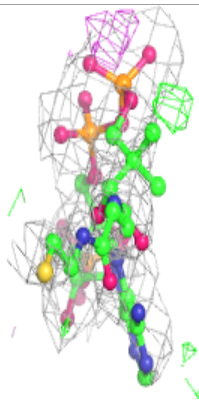


Electron density around COA A 300:

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

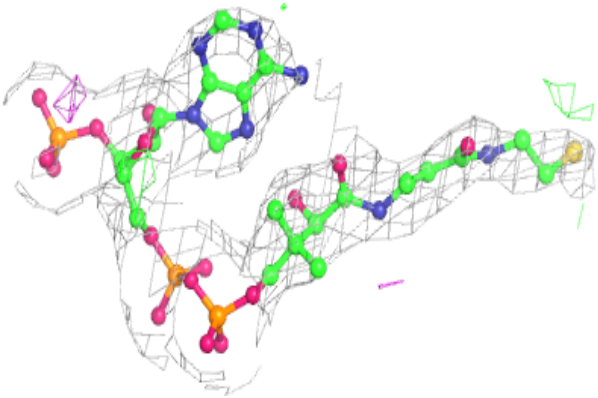


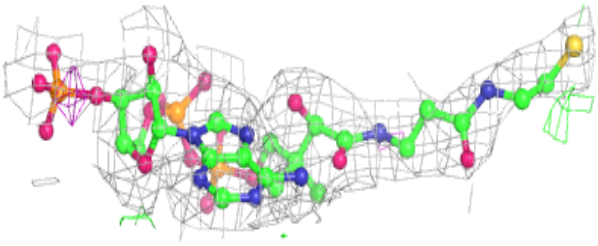


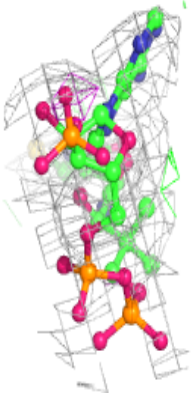


Electron density around COA C 700:

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

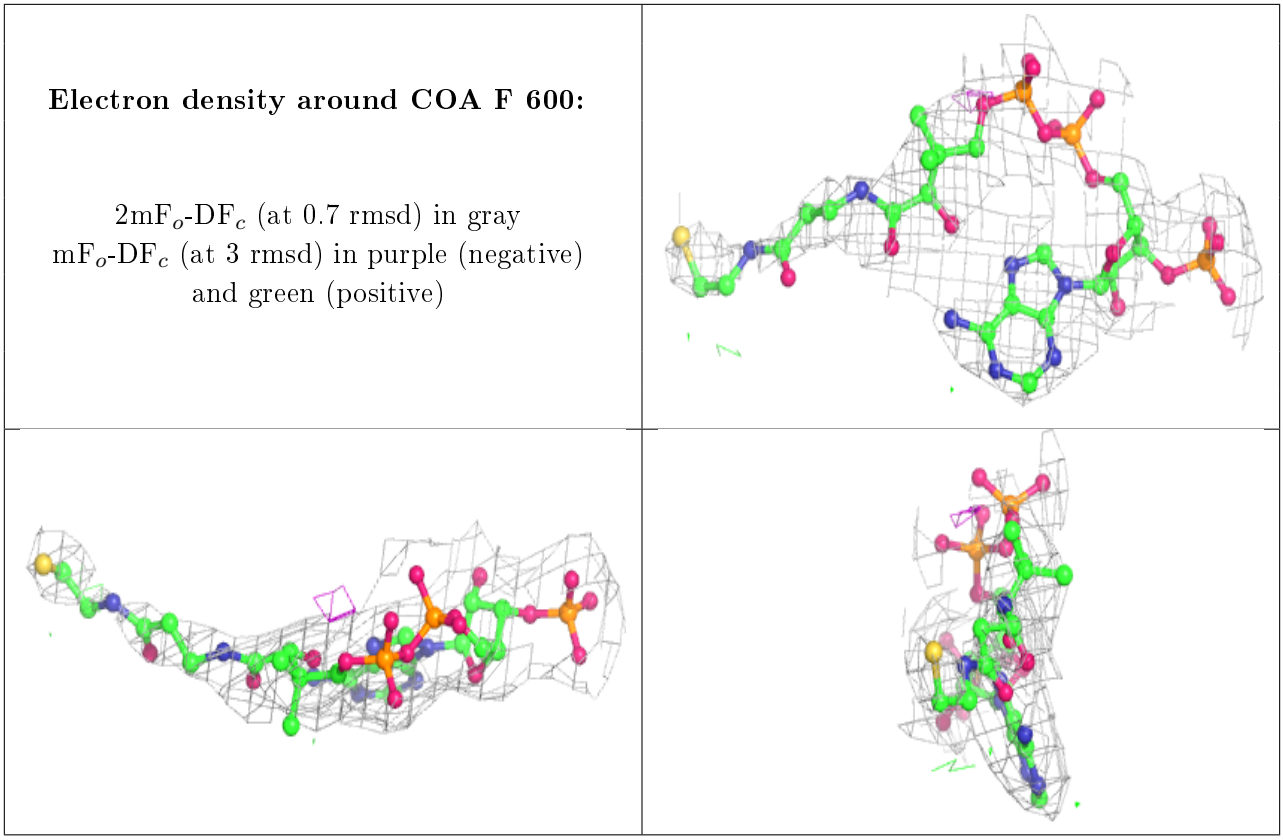






Electron density around COA F 600:

$2mF_o$-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

There are no such residues in this entry.