Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:47 pm BST

PDB ID	:	1KHR
Title	:	Crystal Structure of Vat(D) in Complex with Virginiamycin and Coenzyme A
Authors	:	Sugantino, M.; Roderick, S.L.
Deposited on	:	2001-11-30
Resolution	:	2.80 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:

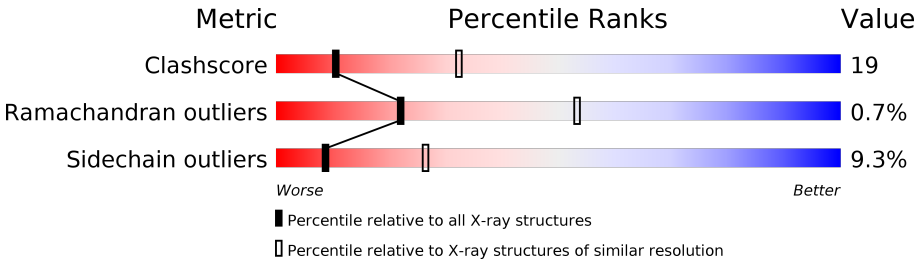
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	209	59% 36%
1	B	209	72% 22%
1	C	209	64% 32%
1	D	209	57% 34% 8%
1	E	209	56% 37%
1	F	209	63% 32%

2 Entry composition

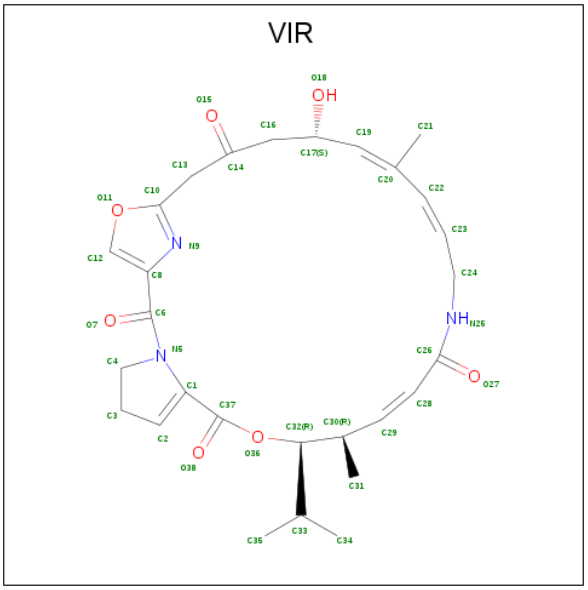
There are 4 unique types of molecules in this entry. The entry contains 10192 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 STREPTOGRAMIN A ACETYLTRANSFERASE.

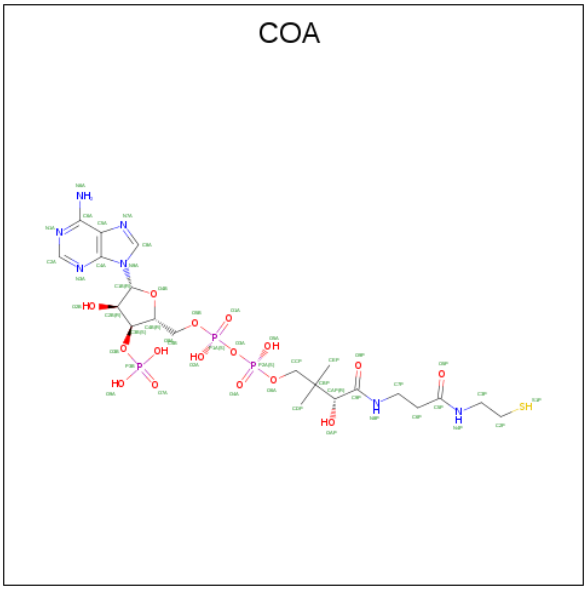
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1611	1037	265	300	9			
1	B	205	Total	C	N	O	S	0	0	0
			1609	1036	265	299	9			
1	C	206	Total	C	N	O	S	0	0	0
			1618	1041	266	302	9			
1	D	206	Total	C	N	O	S	0	0	0
			1622	1046	267	300	9			
1	E	204	Total	C	N	O	S	0	0	0
			1606	1034	264	300	8			
1	F	206	Total	C	N	O	S	0	0	0
			1612	1038	267	298	9			

- Molecule 2 is VIRGINIAMYCIN M1 (three-letter code: VIR) (formula: $C_{28}H_{35}N_3O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			38	28	3	7		
2	A	1	Total	C	N	O	0	0
			38	28	3	7		
2	E	1	Total	C	N	O	0	0
			38	28	3	7		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	22	Total O 22 22	0	0
4	C	16	Total O 16 16	0	0
4	D	23	Total O 23 23	0	0
4	E	23	Total O 23 23	0	0
4	F	13	Total O 13 13	0	0

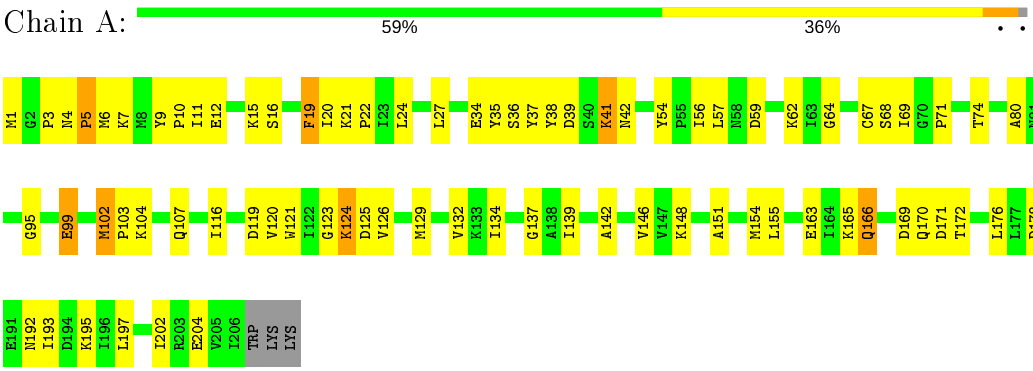
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

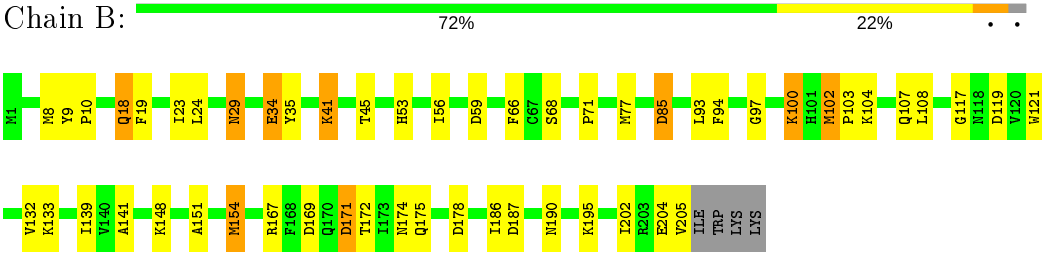
- Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE

Chain A:



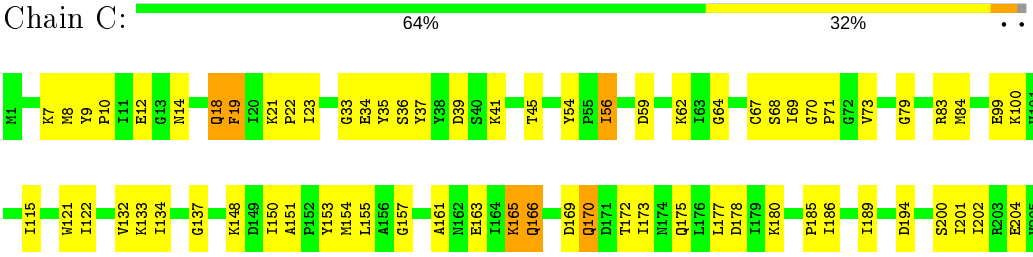
- Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE

Chain B:



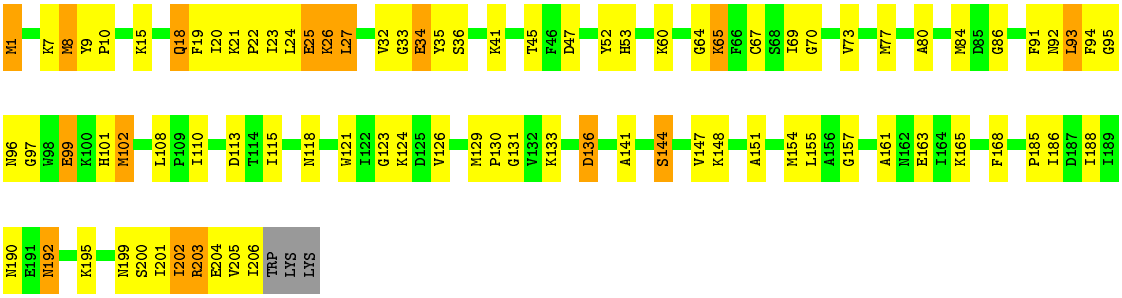
- Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE

Chain C:



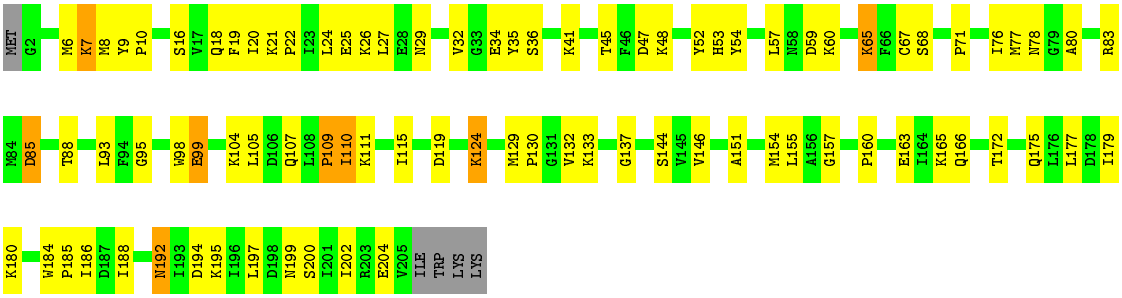
- Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE

Chain D:



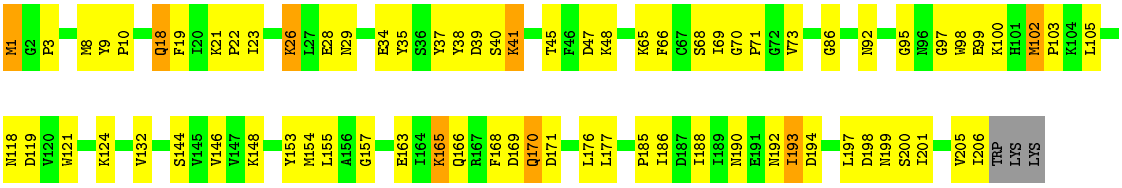
- Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE

Chain E:



- Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE

Chain F:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	186.10Å 185.90Å 186.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 2.80	Depositor
% Data completeness (in resolution range)	91.4 (99.00-2.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.186 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10192	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.39	0/1650	0.65	0/2242
1	B	0.41	0/1648	0.69	0/2238
1	C	0.41	0/1657	0.68	0/2250
1	D	0.40	0/1661	0.64	0/2254
1	E	0.39	0/1645	0.68	0/2234
1	F	0.39	0/1651	0.68	1/2241 (0.0%)
All	All	0.40	0/9912	0.67	1/13459 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	166	GLN	N-CA-C	-5.86	95.17	111.00

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	1611	0	1581	75	0
1	B	1609	0	1585	43	0
1	C	1618	0	1591	47	0
1	D	1622	0	1612	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1606	0	1582	64	0
1	F	1612	0	1590	49	0
2	A	76	0	67	20	0
2	E	38	0	33	7	0
3	A	48	0	32	4	0
3	B	48	0	32	1	0
3	C	48	0	32	8	0
3	D	48	0	32	11	0
3	E	48	0	32	2	0
3	F	48	0	32	2	0
4	A	15	0	0	5	0
4	B	22	0	0	4	0
4	C	16	0	0	2	0
4	D	23	0	0	1	0
4	E	23	0	0	3	0
4	F	13	0	0	0	0
All	All	10192	0	9833	369	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 19.

All (369) 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:57:LEU:HB3	1:E:110:ILE:HD11	1.25	1.18
1:D:199:ASN:O	1:D:202:ILE:CD1	2.10	0.97
1:A:82:HIS:HE2	3:C:303:COA:HS1	1.03	0.87
1:D:199:ASN:O	1:D:202:ILE:HD11	1.74	0.86
2:A:402:VIR:H311	2:A:402:VIR:H352	1.57	0.85
1:D:202:ILE:H	1:D:202:ILE:HD13	1.40	0.85
1:F:37:TYR:HE2	1:F:68:SER:HG	1.21	0.84
1:C:194:ASP:HB2	4:C:3587:HOH:O	1.81	0.80
1:B:186:ILE:HG12	1:B:190:ASN:ND2	1.97	0.80
1:B:104:LYS:HD3	4:B:3572:HOH:O	1.82	0.77
1:A:3:PRO:HG2	1:B:94:PHE:HB3	1.66	0.77
1:E:48:LYS:HE2	4:E:3594:HOH:O	1.85	0.76
1:B:23:ILE:HG22	1:B:24:LEU:HD23	1.66	0.76
1:E:204:GLU:OE1	1:E:204:GLU:HA	1.85	0.75
1:D:95:GLY:HA2	1:D:99:GLU:HG3	1.68	0.75
1:D:121:TRP:HE1	3:D:304:COA:H21	1.51	0.74
1:B:186:ILE:HG12	1:B:190:ASN:HD21	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:MET:HE2	1:A:163:GLU:HG2	1.69	0.74
1:D:93:LEU:O	1:D:93:LEU:HG	1.88	0.74
2:A:402:VIR:C37	2:A:402:VIR:C28	2.67	0.73
1:D:115:ILE:HD12	1:D:133:LYS:HE2	1.70	0.73
1:A:151:ALA:HB3	1:A:154:MET:HG3	1.71	0.71
1:B:10:PRO:HG3	1:B:19:PHE:CD1	2.26	0.71
1:E:175:GLN:O	1:E:179:ILE:HG13	1.91	0.70
1:E:110:ILE:HG22	1:E:110:ILE:O	1.89	0.70
1:C:151:ALA:HB3	1:C:154:MET:HG3	1.74	0.69
1:A:139:ILE:HB	1:A:155:LEU:HD12	1.75	0.69
1:C:155:LEU:HD11	3:C:303:COA:H132	1.74	0.69
1:F:95:GLY:HA2	1:F:99:GLU:HG3	1.73	0.69
1:D:19:PHE:O	1:D:22:PRO:HD2	1.93	0.67
1:D:199:ASN:O	1:D:202:ILE:HD13	1.95	0.67
1:D:24:LEU:O	1:D:27:LEU:HB2	1.95	0.67
1:F:155:LEU:HD11	3:F:306:COA:H132	1.77	0.67
1:B:121:TRP:HE1	3:B:302:COA:H21	1.60	0.66
1:A:95:GLY:HA2	1:A:99:GLU:HG2	1.77	0.66
1:C:10:PRO:HG3	1:C:19:PHE:CD1	2.31	0.66
1:D:202:ILE:HG12	1:D:203:ARG:H	1.60	0.66
2:E:403:VIR:C28	2:E:403:VIR:C2	2.74	0.65
1:D:186:ILE:HD11	1:E:98:TRP:HZ2	1.59	0.65
2:A:401:VIR:H213	3:A:301:COA:S1P	2.37	0.65
1:D:10:PRO:HG3	1:D:19:PHE:CD1	2.31	0.65
1:E:35:TYR:CZ	1:E:186:ILE:HD12	2.31	0.65
2:A:402:VIR:C4	2:A:402:VIR:N9	2.58	0.64
1:C:33:GLY:HA3	1:C:64:GLY:O	1.96	0.64
1:F:121:TRP:HE1	3:F:306:COA:H21	1.62	0.64
1:E:155:LEU:HD11	3:E:305:COA:H132	1.80	0.64
2:A:402:VIR:H311	2:A:402:VIR:C35	2.20	0.64
2:A:401:VIR:H162	1:B:93:LEU:HD21	1.79	0.64
1:E:185:PRO:HD2	1:E:188:ILE:HD12	1.79	0.64
1:D:195:LYS:HD3	1:D:204:GLU:HG3	1.80	0.63
2:A:401:VIR:HC2	2:A:401:VIR:H28	1.81	0.63
1:B:35:TYR:OH	1:B:186:ILE:HD12	1.98	0.63
1:E:57:LEU:HB3	1:E:110:ILE:CD1	2.16	0.63
1:D:202:ILE:HD13	1:D:202:ILE:N	2.13	0.63
1:A:41:LYS:HB2	1:A:71:PRO:HB2	1.80	0.63
1:C:204:GLU:OE1	1:C:204:GLU:HA	1.98	0.63
1:E:20:ILE:HG22	1:E:32:VAL:HG11	1.81	0.62
1:A:41:LYS:O	1:A:41:LYS:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:ILE:O	1:F:26:LYS:HE3	1.99	0.62
2:A:401:VIR:H352	2:A:401:VIR:H311	1.81	0.62
1:A:139:ILE:HB	1:A:155:LEU:CD1	2.29	0.62
1:B:10:PRO:HG3	1:B:19:PHE:CE1	2.35	0.62
1:B:141:ALA:HB1	4:B:3577:HOH:O	1.99	0.62
1:D:202:ILE:HG12	1:D:203:ARG:N	2.14	0.62
1:C:121:TRP:HE1	3:C:303:COA:H21	1.65	0.61
2:E:403:VIR:C37	2:E:403:VIR:C28	2.77	0.61
1:E:20:ILE:CG2	1:E:32:VAL:HG11	2.30	0.61
1:E:83:ARG:HG2	4:E:3510:HOH:O	1.99	0.61
1:A:120:VAL:HG21	4:A:3533:HOH:O	2.00	0.61
1:D:20:ILE:HG23	1:D:24:LEU:HG	1.83	0.61
1:C:37:TYR:CE2	1:C:68:SER:HA	2.36	0.60
1:A:132:VAL:HG11	1:A:146:VAL:HG12	1.82	0.60
1:E:129:MET:O	1:E:132:VAL:HG23	2.01	0.60
1:B:97:GLY:O	1:B:100:LYS:HG3	2.02	0.60
1:B:151:ALA:HB3	1:B:154:MET:HG3	1.84	0.60
1:C:178:ASP:O	1:C:180:LYS:HG3	2.02	0.59
1:F:41:LYS:HB2	1:F:71:PRO:HB2	1.82	0.59
1:B:102:MET:HG3	1:B:103:PRO:CD	2.32	0.59
1:D:70:GLY:CA	3:D:304:COA:H22	2.32	0.59
1:A:3:PRO:CG	1:B:94:PHE:HB3	2.31	0.59
1:A:80:ALA:HA	2:A:402:VIR:H211	1.85	0.58
1:C:21:LYS:HB3	1:C:22:PRO:HD3	1.83	0.58
3:D:304:COA:O9P	3:D:304:COA:H131	2.03	0.58
1:F:154:MET:HE3	1:F:163:GLU:HB3	1.86	0.58
1:F:169:ASP:OD1	1:F:171:ASP:HB3	2.02	0.58
1:D:144:SER:OG	1:D:157:GLY:HA2	2.04	0.58
1:E:71:PRO:HG2	1:E:124:LYS:HB2	1.85	0.58
1:A:134:ILE:HG22	4:A:3533:HOH:O	2.03	0.58
1:F:35:TYR:OH	1:F:186:ILE:HD12	2.04	0.58
4:B:3511:HOH:O	1:C:83:ARG:HG2	2.02	0.58
1:B:102:MET:HG3	1:B:103:PRO:HD2	1.84	0.57
1:E:115:ILE:HD12	1:E:133:LYS:HE2	1.85	0.57
1:D:186:ILE:HD11	1:E:98:TRP:CZ2	2.39	0.57
1:D:36:SER:HB3	1:D:67:CYS:HB2	1.86	0.57
1:D:70:GLY:HA3	3:D:304:COA:H22	1.85	0.57
1:A:195:LYS:HZ2	1:A:204:GLU:HG3	1.70	0.57
1:A:195:LYS:NZ	1:A:204:GLU:CD	2.58	0.56
1:D:155:LEU:HD11	3:D:304:COA:H132	1.87	0.56
3:D:304:COA:C2A	1:E:160:PRO:HG3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ILE:HG12	1:C:122:ILE:HD12	1.87	0.56
1:E:186:ILE:HD11	1:F:98:TRP:HZ2	1.70	0.56
1:D:204:GLU:OE1	1:D:204:GLU:HA	2.06	0.56
1:A:169:ASP:OD1	1:A:171:ASP:HB3	2.06	0.56
1:A:54:TYR:CE1	2:A:402:VIR:HC32	2.40	0.56
2:A:402:VIR:N9	2:A:402:VIR:HC41	2.19	0.55
1:B:174:ASN:O	1:B:178:ASP:HB2	2.06	0.55
1:C:19:PHE:O	1:C:22:PRO:HD2	2.06	0.55
1:D:154:MET:HE2	1:D:163:GLU:HG2	1.89	0.55
1:C:172:THR:O	1:C:175:GLN:HB2	2.06	0.55
1:E:25:GLU:C	1:E:27:LEU:H	2.10	0.55
1:B:169:ASP:OD1	1:B:171:ASP:CB	2.55	0.55
1:D:205:VAL:HG12	1:D:205:VAL:O	2.07	0.54
1:D:25:GLU:C	1:D:27:LEU:H	2.11	0.54
1:A:129:MET:O	1:A:132:VAL:HG23	2.07	0.54
1:C:169:ASP:O	1:C:170:GLN:C	2.44	0.54
1:D:151:ALA:HB3	1:D:154:MET:HG3	1.89	0.54
1:E:8:MET:HE2	1:E:9:TYR:CE1	2.42	0.54
1:A:195:LYS:HZ3	1:A:204:GLU:CD	2.10	0.54
1:A:82:HIS:NE2	3:C:303:COA:S1P	2.58	0.54
1:F:21:LYS:HB3	1:F:22:PRO:HD3	1.89	0.54
1:D:200:SER:O	1:D:204:GLU:HG2	2.07	0.54
1:C:172:THR:HG23	1:C:202:ILE:CD1	2.39	0.53
1:B:139:ILE:HG13	1:B:167:ARG:HD2	1.89	0.53
1:C:134:ILE:HG23	1:C:150:ILE:HB	1.90	0.53
1:E:36:SER:HB3	1:E:67:CYS:HB2	1.91	0.53
1:C:165:LYS:HG2	1:C:166:GLN:N	2.22	0.53
1:F:185:PRO:HD2	1:F:188:ILE:HD12	1.89	0.53
1:E:132:VAL:HG11	1:E:146:VAL:HG12	1.89	0.53
1:C:8:MET:HE2	1:C:23:ILE:HD11	1.90	0.53
1:F:144:SER:OG	1:F:157:GLY:HA2	2.09	0.53
1:F:97:GLY:N	1:F:99:GLU:OE2	2.37	0.53
1:D:52:TYR:CD1	1:D:80:ALA:HB2	2.45	0.52
1:A:95:GLY:HA2	1:A:99:GLU:CG	2.40	0.52
1:A:192:ASN:O	1:A:195:LYS:N	2.43	0.52
1:C:115:ILE:HD12	1:C:133:LYS:HE2	1.90	0.52
1:D:97:GLY:N	1:D:99:GLU:OE2	2.39	0.52
2:E:403:VIR:C28	2:E:403:VIR:HC2	2.38	0.52
1:A:132:VAL:HG11	1:A:146:VAL:CG1	2.40	0.52
1:B:169:ASP:OD1	1:B:171:ASP:HB2	2.10	0.52
1:D:201:ILE:O	1:D:205:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:66:PHE:O	1:F:119:ASP:HA	2.10	0.52
1:C:121:TRP:CZ2	3:C:303:COA:H71	2.45	0.52
1:C:154:MET:HE2	1:C:163:GLU:HG2	1.92	0.52
1:C:39:ASP:O	1:C:71:PRO:HB3	2.10	0.52
1:E:151:ALA:HB3	1:E:154:MET:HG3	1.91	0.52
3:D:304:COA:H2A	1:E:160:PRO:HG3	1.91	0.51
2:A:401:VIR:H19	1:B:93:LEU:CD2	2.39	0.51
1:A:36:SER:HB3	1:A:67:CYS:HB2	1.91	0.51
1:A:4:ASN:O	1:A:6:MET:N	2.44	0.51
1:E:52:TYR:CD1	1:E:80:ALA:HB2	2.45	0.51
1:A:82:HIS:CD2	3:C:303:COA:HS1	2.25	0.51
1:D:91:PHE:HD1	1:F:197:LEU:HD21	1.76	0.51
1:F:38:TYR:CE2	1:F:40:SER:HA	2.45	0.51
1:F:39:ASP:O	1:F:71:PRO:HB3	2.11	0.51
2:E:403:VIR:C4	2:E:403:VIR:N9	2.73	0.50
1:D:147:VAL:HG23	1:D:148:LYS:HG2	1.93	0.50
1:D:94:PHE:HB3	1:F:3:PRO:HG3	1.93	0.50
1:E:78:ASN:OD1	1:E:111:LYS:N	2.45	0.50
1:F:170:GLN:HA	1:F:170:GLN:NE2	2.25	0.50
1:E:26:LYS:O	1:E:27:LEU:HD23	2.12	0.50
1:B:195:LYS:NZ	1:B:204:GLU:HG3	2.26	0.50
1:A:104:LYS:O	1:A:107:GLN:N	2.39	0.49
1:B:175:GLN:NE2	1:B:202:ILE:CG2	2.75	0.49
1:B:18:GLN:OE1	1:B:45:THR:HA	2.12	0.49
1:A:195:LYS:NZ	1:A:204:GLU:HG3	2.27	0.49
1:F:132:VAL:HG11	1:F:146:VAL:HG12	1.94	0.49
1:E:45:THR:OG1	4:E:3594:HOH:O	2.20	0.49
1:E:95:GLY:HA2	1:E:99:GLU:HG3	1.95	0.49
1:A:119:ASP:O	1:A:137:GLY:HA2	2.13	0.48
1:A:20:ILE:CD1	1:A:69:ILE:HD12	2.43	0.48
3:C:303:COA:H1B	4:C:3606:HOH:O	2.13	0.48
1:C:177:LEU:O	1:C:180:LYS:HG2	2.13	0.48
1:E:7:LYS:O	1:E:19:PHE:HB2	2.13	0.48
1:A:176:LEU:HG	1:A:202:ILE:HD11	1.96	0.48
1:C:70:GLY:O	1:C:73:VAL:HG23	2.13	0.48
1:D:23:ILE:O	1:D:26:LYS:HG3	2.12	0.48
1:F:153:TYR:CE2	1:F:176:LEU:HD13	2.49	0.48
1:B:129:MET:O	1:B:132:VAL:HG23	2.12	0.48
1:A:37:TYR:CE2	1:A:68:SER:HA	2.47	0.48
1:C:166:GLN:HG2	1:C:173:ILE:CD1	2.43	0.48
2:E:403:VIR:C28	2:E:403:VIR:C1	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:VIR:H19	1:B:93:LEU:HD22	1.95	0.48
1:F:92:ASN:HA	1:F:98:TRP:O	2.13	0.48
1:D:34:GLU:HG2	1:D:65:LYS:HD2	1.96	0.48
1:E:195:LYS:HD2	1:E:204:GLU:HG3	1.95	0.48
1:F:192:ASN:O	1:F:193:ILE:C	2.53	0.48
1:A:35:TYR:CZ	1:A:186:ILE:HD13	2.49	0.47
1:D:84:MET:C	1:D:86:GLY:H	2.16	0.47
1:E:154:MET:CE	1:E:163:GLU:HB3	2.44	0.47
1:A:56:ILE:HG23	1:A:57:LEU:HD23	1.96	0.47
1:C:165:LYS:HG2	1:C:166:GLN:O	2.15	0.47
1:E:154:MET:HE3	1:E:163:GLU:HB3	1.96	0.47
1:E:35:TYR:OH	1:E:186:ILE:HD12	2.14	0.47
1:A:11:ILE:HG22	1:A:12:GLU:N	2.28	0.47
1:A:99:GLU:HG3	1:A:99:GLU:H	1.25	0.47
1:E:104:LYS:O	1:E:105:LEU:C	2.53	0.47
1:C:102:MET:HG3	1:C:103:PRO:HD2	1.95	0.47
1:C:172:THR:HG23	1:C:202:ILE:HD11	1.95	0.47
1:B:204:GLU:O	1:B:205:VAL:C	2.53	0.47
1:D:141:ALA:HA	3:D:304:COA:O9P	2.14	0.47
1:F:28:GLU:O	1:F:29:ASN:HB2	2.14	0.47
1:A:195:LYS:CD	1:A:204:GLU:HG3	2.45	0.47
1:A:20:ILE:HG23	1:A:24:LEU:HG	1.97	0.47
1:D:113:ASP:O	1:D:131:GLY:HA2	2.14	0.47
1:E:107:GLN:O	1:E:109:PRO:HD3	2.15	0.47
1:E:29:ASN:HB3	1:E:60:LYS:HG3	1.97	0.47
1:F:10:PRO:HB3	1:F:19:PHE:CE1	2.50	0.47
1:E:104:LYS:O	1:E:107:GLN:N	2.36	0.47
1:E:197:LEU:O	1:F:86:GLY:HA3	2.14	0.47
1:B:66:PHE:O	1:B:119:ASP:HA	2.15	0.46
1:B:172:THR:HG23	1:B:202:ILE:CD1	2.45	0.46
1:C:137:GLY:O	1:C:153:TYR:HA	2.16	0.46
1:E:83:ARG:HE	1:E:85:ASP:CG	2.19	0.46
1:D:10:PRO:HG3	1:D:19:PHE:CE1	2.50	0.46
1:A:83:ARG:HG2	4:A:3526:HOH:O	2.16	0.46
1:D:7:LYS:HE2	1:D:9:TYR:O	2.16	0.46
1:E:54:TYR:CE1	2:E:403:VIR:HC32	2.50	0.46
1:E:119:ASP:O	1:E:137:GLY:HA2	2.16	0.46
1:E:54:TYR:HE1	2:E:403:VIR:HC32	1.81	0.46
2:A:401:VIR:H23	2:A:401:VIR:H211	1.63	0.46
1:D:129:MET:HB3	1:D:130:PRO:CD	2.46	0.46
1:F:1:MET:HE3	1:F:190:ASN:CG	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:GLU:HG2	1:E:65:LYS:HD2	1.98	0.46
1:A:39:ASP:O	1:A:71:PRO:HB3	2.16	0.45
1:E:144:SER:OG	1:E:157:GLY:HA2	2.15	0.45
1:E:8:MET:HB3	1:E:8:MET:HE3	1.79	0.45
1:D:35:TYR:CZ	1:D:186:ILE:HD12	2.50	0.45
1:A:20:ILE:HD11	1:A:69:ILE:HD12	1.98	0.45
1:D:185:PRO:HD2	1:D:188:ILE:HD12	1.99	0.45
1:A:59:ASP:OD1	1:A:59:ASP:N	2.48	0.45
1:C:36:SER:HB3	1:C:67:CYS:HB2	1.98	0.45
1:F:1:MET:HB3	1:F:190:ASN:ND2	2.32	0.45
1:C:200:SER:O	1:C:202:ILE:N	2.49	0.45
1:E:53:HIS:CD2	1:E:77:MET:HG3	2.51	0.45
1:E:59:ASP:N	1:E:59:ASP:OD1	2.47	0.45
1:D:20:ILE:CG2	1:D:24:LEU:HG	2.47	0.45
1:F:170:GLN:NE2	1:F:170:GLN:CA	2.79	0.45
1:A:151:ALA:HB3	1:A:154:MET:CG	2.42	0.45
1:A:38:TYR:HD1	1:A:69:ILE:HG22	1.82	0.45
1:A:102:MET:HG3	1:A:103:PRO:HD2	1.97	0.45
1:D:95:GLY:O	1:D:96:ASN:HB2	2.17	0.45
1:B:59:ASP:N	1:B:59:ASP:OD1	2.49	0.44
1:A:134:ILE:CG2	4:A:3533:HOH:O	2.63	0.44
1:B:186:ILE:HG23	1:B:187:ASP:N	2.32	0.44
1:C:200:SER:C	1:C:202:ILE:N	2.71	0.44
1:D:108:LEU:O	1:D:110:ILE:HG13	2.18	0.44
1:D:118:ASN:O	1:D:136:ASP:HB3	2.17	0.44
1:D:18:GLN:OE1	1:D:45:THR:HA	2.17	0.44
1:D:192:ASN:N	1:D:192:ASN:ND2	2.65	0.44
1:E:99:GLU:HG3	1:E:99:GLU:H	1.39	0.44
1:D:20:ILE:HD11	1:D:69:ILE:HD12	1.98	0.44
1:D:121:TRP:NE1	3:D:304:COA:H21	2.25	0.44
1:E:200:SER:C	1:E:202:ILE:H	2.21	0.44
1:B:8:MET:HE3	1:B:9:TYR:CE1	2.53	0.44
1:D:123:GLY:O	1:D:126:VAL:HG23	2.18	0.44
1:D:91:PHE:CD1	1:F:197:LEU:HD21	2.53	0.44
1:B:104:LYS:O	1:B:107:GLN:HB2	2.17	0.44
1:D:34:GLU:HG2	1:D:34:GLU:H	1.51	0.44
1:C:137:GLY:HA3	1:C:153:TYR:CE2	2.53	0.44
1:D:157:GLY:O	1:D:161:ALA:HA	2.17	0.44
1:E:24:LEU:HD23	1:E:47:ASP:HB3	1.99	0.44
1:A:123:GLY:O	1:A:126:VAL:HG23	2.18	0.44
1:C:132:VAL:HG12	1:C:133:LYS:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:GLY:O	1:C:161:ALA:HA	2.18	0.44
1:C:18:GLN:OE1	1:C:45:THR:HA	2.18	0.44
1:A:116:ILE:HG12	1:A:134:ILE:HD12	2.00	0.43
1:A:195:LYS:HD3	1:A:204:GLU:HG3	2.00	0.43
1:B:195:LYS:HZ2	1:B:204:GLU:HG3	1.83	0.43
1:E:188:ILE:O	1:E:192:ASN:ND2	2.50	0.43
1:B:53:HIS:CG	1:B:77:MET:HG3	2.54	0.43
1:C:14:ASN:C	1:C:14:ASN:OD1	2.57	0.43
1:E:179:ILE:HG22	1:E:184:TRP:CZ2	2.53	0.43
2:A:402:VIR:H213	3:C:303:COA:S1P	2.58	0.43
1:D:205:VAL:O	1:D:206:ILE:CB	2.65	0.43
1:D:99:GLU:C	1:D:101:HIS:H	2.22	0.43
1:E:10:PRO:HB3	1:E:19:PHE:CE1	2.53	0.43
2:A:401:VIR:C35	2:A:401:VIR:H311	2.43	0.43
1:A:165:LYS:HG2	1:A:166:GLN:O	2.17	0.43
1:A:35:TYR:CE1	1:A:186:ILE:HD13	2.53	0.43
1:D:20:ILE:CD1	1:D:69:ILE:HD12	2.48	0.43
1:B:8:MET:CE	1:B:9:TYR:CE1	3.02	0.43
1:C:59:ASP:OD1	1:C:59:ASP:N	2.45	0.43
1:D:1:MET:HB3	1:D:190:ASN:ND2	2.34	0.43
1:D:188:ILE:O	1:D:192:ASN:ND2	2.51	0.43
1:D:53:HIS:CG	1:D:77:MET:HG3	2.53	0.43
1:A:10:PRO:HB3	1:A:19:PHE:CE1	2.54	0.43
1:A:24:LEU:O	1:A:27:LEU:HB2	2.19	0.43
1:C:132:VAL:CG1	1:C:133:LYS:N	2.82	0.43
1:D:8:MET:HG2	1:D:22:PRO:HB2	2.00	0.43
1:F:37:TYR:CE2	1:F:68:SER:HA	2.54	0.43
1:E:21:LYS:HB3	1:E:22:PRO:CD	2.48	0.43
1:A:4:ASN:C	1:A:6:MET:H	2.22	0.43
3:D:304:COA:H4B	3:D:304:COA:O7A	2.19	0.43
1:D:53:HIS:CD2	1:D:77:MET:HG3	2.54	0.43
1:A:21:LYS:HB3	1:A:22:PRO:CD	2.48	0.42
2:A:402:VIR:C37	2:A:402:VIR:O7	2.64	0.42
1:D:186:ILE:HD13	4:D:3588:HOH:O	2.19	0.42
1:E:132:VAL:HG12	1:E:133:LYS:N	2.34	0.42
1:F:205:VAL:O	1:F:206:ILE:C	2.57	0.42
1:A:9:TYR:CD2	1:A:15:LYS:HA	2.53	0.42
1:F:34:GLU:HG2	1:F:65:LYS:HE2	2.00	0.42
1:E:177:LEU:O	1:E:180:LYS:HG3	2.18	0.42
1:B:85:ASP:HB2	4:B:3568:HOH:O	2.18	0.42
1:C:154:MET:HE2	1:C:163:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:NZ	1:A:204:GLU:CG	2.82	0.42
2:A:402:VIR:H352	2:A:402:VIR:C31	2.34	0.42
1:D:21:LYS:HB3	1:D:22:PRO:HD3	2.00	0.42
1:A:36:SER:HA	1:A:67:CYS:H	1.85	0.42
1:B:132:VAL:HG12	1:B:133:LYS:N	2.35	0.42
1:B:34:GLU:HB2	1:B:35:TYR:CD1	2.55	0.42
1:C:56:ILE:O	1:C:56:ILE:HG13	2.18	0.42
1:F:192:ASN:O	1:F:194:ASP:N	2.52	0.42
1:A:85:ASP:OD1	1:A:85:ASP:N	2.51	0.42
1:D:33:GLY:HA3	1:D:64:GLY:O	2.19	0.42
2:A:401:VIR:H28	2:A:401:VIR:C2	2.48	0.42
1:E:76:ILE:HG22	1:E:130:PRO:HG3	2.02	0.42
1:A:193:ILE:O	1:A:197:LEU:HG	2.18	0.42
1:A:27:LEU:HA	1:A:27:LEU:HD23	1.69	0.42
1:B:29:ASN:O	1:B:29:ASN:OD1	2.37	0.42
1:D:92:ASN:HB2	1:D:102:MET:HE2	2.02	0.42
1:E:172:THR:HG23	1:E:202:ILE:HD13	2.02	0.42
1:E:21:LYS:HB3	1:E:22:PRO:HD3	2.02	0.42
1:C:54:TYR:CE1	1:C:79:GLY:HA3	2.55	0.41
3:D:304:COA:O9P	3:D:304:COA:CDP	2.67	0.41
1:D:36:SER:CB	1:D:67:CYS:HB2	2.50	0.41
1:F:188:ILE:O	1:F:192:ASN:ND2	2.43	0.41
1:F:198:ASP:OD1	1:F:200:SER:HB3	2.20	0.41
1:B:85:ASP:OD1	1:B:85:ASP:N	2.47	0.41
1:E:179:ILE:O	1:E:180:LYS:HB2	2.21	0.41
1:F:132:VAL:HG11	1:F:146:VAL:CG1	2.50	0.41
3:E:305:COA:H4B	3:E:305:COA:O7A	2.20	0.41
1:F:154:MET:SD	1:F:165:LYS:O	2.79	0.41
1:F:47:ASP:OD2	1:F:48:LYS:NZ	2.53	0.41
1:A:192:ASN:O	1:A:193:ILE:C	2.58	0.41
1:A:4:ASN:HA	1:A:5:PRO:HD2	1.83	0.41
1:D:20:ILE:HG22	1:D:32:VAL:HG11	2.01	0.41
1:F:198:ASP:OD1	1:F:198:ASP:C	2.59	0.41
1:F:168:PHE:CZ	1:F:199:ASN:ND2	2.89	0.41
1:C:35:TYR:OH	1:C:186:ILE:CD1	2.69	0.41
1:A:11:ILE:CG2	1:A:12:GLU:N	2.83	0.41
1:C:7:LYS:HE2	1:C:9:TYR:O	2.20	0.41
1:D:73:VAL:HA	1:D:126:VAL:O	2.21	0.41
1:F:99:GLU:H	1:F:99:GLU:CD	2.23	0.41
2:A:402:VIR:O38	2:A:402:VIR:C28	2.69	0.41
1:F:102:MET:HG3	1:F:103:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:GLY:O	1:F:73:VAL:HG23	2.21	0.41
1:A:9:TYR:HA	1:A:10:PRO:HD2	1.89	0.40
1:A:120:VAL:CG2	4:A:3533:HOH:O	2.66	0.40
1:B:108:LEU:HD23	1:B:108:LEU:HA	1.81	0.40
1:E:35:TYR:CE1	1:E:186:ILE:HD12	2.56	0.40
1:E:95:GLY:HA2	1:E:99:GLU:CG	2.51	0.40
1:A:121:TRP:HE1	3:A:301:COA:H21	1.86	0.40
1:A:124:LYS:NZ	1:A:125:ASP:OD2	2.42	0.40
1:A:186:ILE:O	1:A:190:ASN:HB2	2.21	0.40
1:F:9:TYR:HA	1:F:10:PRO:HD2	1.89	0.40
1:A:121:TRP:CZ2	3:A:301:COA:H71	2.57	0.40
1:A:142:ALA:HB2	3:A:301:COA:O5P	2.21	0.40
1:B:41:LYS:HB2	1:B:71:PRO:HB2	2.03	0.40
1:D:70:GLY:O	1:D:73:VAL:HG23	2.21	0.40
1:A:172:THR:HG23	1:A:202:ILE:CD1	2.51	0.40
1:C:10:PRO:HG3	1:C:19:PHE:CE1	2.55	0.40
1:C:185:PRO:O	1:C:189:ILE:HG13	2.21	0.40
1:D:26:LYS:O	1:D:27:LEU:HD23	2.21	0.40
1:F:177:LEU:HD23	1:F:177:LEU:HA	1.83	0.40
1:F:38:TYR:HD1	1:F:69:ILE:HG22	1.87	0.40
1:A:154:MET:HE2	1:A:163:GLU:CG	2.46	0.40
1:A:1:MET:HB3	1:A:190:ASN:HD21	1.86	0.40
1:D:204:GLU:OE1	1:D:204:GLU:CA	2.70	0.40
1:F:18:GLN:OE1	1:F:45:THR:HA	2.21	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	204/209 (98%)	188 (92%)	13 (6%)	3 (2%)	10 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	203/209 (97%)	192 (95%)	10 (5%)	1 (0%)	29 61
1	C	204/209 (98%)	190 (93%)	12 (6%)	2 (1%)	15 44
1	D	204/209 (98%)	186 (91%)	18 (9%)	0	100 100
1	E	202/209 (97%)	181 (90%)	20 (10%)	1 (0%)	29 61
1	F	204/209 (98%)	189 (93%)	14 (7%)	1 (0%)	29 61
All	All	1221/1254 (97%)	1126 (92%)	87 (7%)	8 (1%)	22 53

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	34	GLU
1	A	64	GLY
1	E	109	PRO
1	A	5	PRO
1	A	42	ASN
1	B	117	GLY
1	C	201	ILE
1	F	193	ILE

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	173/183 (94%)	158 (91%)	15 (9%)	10 30
1	B	173/183 (94%)	160 (92%)	13 (8%)	13 37
1	C	174/183 (95%)	160 (92%)	14 (8%)	12 34
1	D	176/183 (96%)	153 (87%)	23 (13%)	4 12
1	E	174/183 (95%)	156 (90%)	18 (10%)	7 21
1	F	173/183 (94%)	159 (92%)	14 (8%)	11 33
All	All	1043/1098 (95%)	946 (91%)	97 (9%)	9 26

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	16	SER
1	A	19	PHE
1	A	34	GLU
1	A	41	LYS
1	A	62	LYS
1	A	74	THR
1	A	85	ASP
1	A	99	GLU
1	A	102	MET
1	A	124	LYS
1	A	148	LYS
1	A	166	GLN
1	A	170	GLN
1	A	178	ASP
1	B	18	GLN
1	B	29	ASN
1	B	34	GLU
1	B	41	LYS
1	B	56	ILE
1	B	68	SER
1	B	85	ASP
1	B	100	LYS
1	B	102	MET
1	B	124	LYS
1	B	148	LYS
1	B	154	MET
1	B	171	ASP
1	C	12	GLU
1	C	18	GLN
1	C	19	PHE
1	C	41	LYS
1	C	56	ILE
1	C	62	LYS
1	C	84	MET
1	C	99	GLU
1	C	100	LYS
1	C	105	LEU
1	C	148	LYS
1	C	165	LYS
1	C	166	GLN
1	C	170	GLN
1	D	1	MET

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Mol	Chain	Res	Type
1	D	8	MET
1	D	15	LYS
1	D	18	GLN
1	D	25	GLU
1	D	26	LYS
1	D	27	LEU
1	D	34	GLU
1	D	41	LYS
1	D	47	ASP
1	D	60	LYS
1	D	65	LYS
1	D	93	LEU
1	D	99	GLU
1	D	102	MET
1	D	124	LYS
1	D	136	ASP
1	D	144	SER
1	D	165	LYS
1	D	168	PHE
1	D	192	ASN
1	D	202	ILE
1	D	203	ARG
1	E	6	MET
1	E	7	LYS
1	E	16	SER
1	E	18	GLN
1	E	41	LYS
1	E	65	LYS
1	E	68	SER
1	E	85	ASP
1	E	88	THR
1	E	93	LEU
1	E	99	GLU
1	E	110	ILE
1	E	124	LYS
1	E	165	LYS
1	E	166	GLN
1	E	192	ASN
1	E	194	ASP
1	E	199	ASN
1	F	1	MET
1	F	8	MET

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Mol	Chain	Res	Type
1	F	18	GLN
1	F	26	LYS
1	F	41	LYS
1	F	100	LYS
1	F	102	MET
1	F	105	LEU
1	F	118	ASN
1	F	124	LYS
1	F	148	LYS
1	F	165	LYS
1	F	170	GLN
1	F	201	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	174	ASN
1	B	143	ASN
1	B	174	ASN
1	B	175	GLN
1	C	174	ASN
1	D	166	GLN
1	D	192	ASN
1	E	42	ASN
1	E	58	ASN
1	E	81	ASN
1	E	166	GLN
1	E	170	GLN
1	E	174	ASN
1	E	192	ASN
1	F	143	ASN
1	F	170	GLN
1	F	174	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
3	COA	A	301	-	41,50,50	1.11	1 (2%)	52,75,75	1.39	5 (9%)
2	VIR	E	403	-	34,40,40	2.31	9 (26%)	36,55,55	2.21	8 (22%)
2	VIR	A	402	-	34,40,40	2.40	9 (26%)	36,55,55	2.99	13 (36%)
3	COA	B	302	-	41,50,50	1.32	5 (12%)	52,75,75	1.17	1 (1%)
3	COA	F	306	-	41,50,50	1.31	5 (12%)	52,75,75	1.17	1 (1%)
2	VIR	A	401	-	34,40,40	2.03	7 (20%)	36,55,55	2.75	11 (30%)
3	COA	C	303	-	41,50,50	1.31	5 (12%)	52,75,75	1.17	2 (3%)
3	COA	D	304	-	41,50,50	1.01	1 (2%)	52,75,75	1.59	9 (17%)
3	COA	E	305	-	41,50,50	1.14	2 (4%)	52,75,75	1.33	7 (13%)

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
3	COA	A	301	-	-	10/44/64/64	0/3/3/3
2	VIR	E	403	-	-	11/42/58/58	0/2/3/3
2	VIR	A	402	-	-	19/42/58/58	0/2/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	B	302	-	-	11/44/64/64	0/3/3/3
3	COA	F	306	-	-	11/44/64/64	0/3/3/3
2	VIR	A	401	-	-	10/42/58/58	0/2/3/3
3	COA	C	303	-	-	3/44/64/64	0/3/3/3
3	COA	D	304	-	-	13/44/64/64	0/3/3/3
3	COA	E	305	-	-	11/44/64/64	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	VIR	C28-C29	-8.77	1.11	1.32
2	A	401	VIR	C28-C29	-8.19	1.13	1.32
2	E	403	VIR	C28-C29	-8.05	1.13	1.32
2	E	403	VIR	C1-N5	5.41	1.46	1.39
2	E	403	VIR	C28-C26	5.22	1.59	1.48
2	A	402	VIR	C8-C6	-4.89	1.42	1.50
2	A	402	VIR	C28-C26	4.47	1.57	1.48
2	A	401	VIR	C28-C26	4.00	1.56	1.48
2	A	402	VIR	C6-N5	-3.92	1.30	1.39
2	A	402	VIR	C30-C29	3.66	1.60	1.51
2	E	403	VIR	O36-C32	3.65	1.50	1.44
2	A	401	VIR	C1-N5	3.51	1.44	1.39
2	A	402	VIR	C4-N5	3.32	1.52	1.47
3	A	301	COA	O6A-CCP	2.97	1.53	1.43
2	A	402	VIR	O36-C32	2.95	1.49	1.44
3	C	303	COA	C6P-C5P	2.94	1.56	1.51
3	B	302	COA	C6P-C5P	2.93	1.56	1.51
3	F	306	COA	C6P-C5P	2.90	1.56	1.51
2	E	403	VIR	C13-C14	-2.77	1.46	1.52
3	E	305	COA	C6P-C5P	2.75	1.56	1.51
3	C	303	COA	C3P-N4P	2.72	1.52	1.46
2	E	403	VIR	C8-C6	2.71	1.55	1.50
3	B	302	COA	C3P-N4P	2.70	1.52	1.46
3	F	306	COA	C3P-N4P	2.69	1.52	1.46
2	A	401	VIR	C4-N5	2.63	1.51	1.47
2	A	401	VIR	C13-C14	-2.50	1.47	1.52
3	F	306	COA	O6A-CCP	2.48	1.51	1.43
2	A	402	VIR	C22-C23	2.47	1.38	1.32
3	B	302	COA	O6A-CCP	2.47	1.51	1.43
3	C	303	COA	O6A-CCP	2.45	1.51	1.43
2	A	402	VIR	C30-C32	2.41	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	305	COA	O6A-CCP	2.39	1.51	1.43
3	C	303	COA	C7P-N8P	2.38	1.51	1.46
3	B	302	COA	C7P-N8P	2.34	1.51	1.46
2	E	403	VIR	C16-C17	-2.31	1.50	1.54
3	F	306	COA	C7P-N8P	2.31	1.51	1.46
3	F	306	COA	C2P-S1P	2.25	1.88	1.80
3	B	302	COA	C2P-S1P	2.24	1.88	1.80
3	C	303	COA	C2P-S1P	2.24	1.88	1.80
2	E	403	VIR	C4-N5	2.19	1.50	1.47
3	D	304	COA	O6A-CCP	2.12	1.50	1.43
2	A	401	VIR	C30-C29	2.10	1.56	1.51
2	A	401	VIR	C22-C23	2.09	1.37	1.32
2	E	403	VIR	C22-C23	2.04	1.37	1.32

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	402	VIR	C28-C26-N25	-9.41	97.23	114.97
2	A	401	VIR	C28-C26-N25	-8.89	98.21	114.97
2	E	403	VIR	C28-C26-N25	-7.98	99.93	114.97
2	A	402	VIR	O27-C26-C28	6.66	138.21	123.03
2	A	401	VIR	O27-C26-C28	6.28	137.34	123.03
2	A	401	VIR	O36-C37-C1	-6.03	103.18	110.53
2	E	403	VIR	O27-C26-C28	5.99	136.70	123.03
2	A	402	VIR	C8-C6-N5	-5.60	111.27	118.48
3	A	301	COA	C1B-N9A-C4A	-5.42	117.12	126.64
3	F	306	COA	C1B-N9A-C4A	-5.41	117.14	126.64
3	E	305	COA	C1B-N9A-C4A	-5.40	117.15	126.64
3	B	302	COA	C1B-N9A-C4A	-5.32	117.29	126.64
2	A	402	VIR	C23-C22-C20	-5.32	117.85	125.89
3	C	303	COA	C1B-N9A-C4A	-5.30	117.33	126.64
2	A	402	VIR	O36-C32-C30	5.14	115.68	107.09
3	D	304	COA	C3P-N4P-C5P	-4.71	114.08	122.84
2	A	402	VIR	C30-C29-C28	4.70	139.27	126.44
3	D	304	COA	C1B-N9A-C4A	-4.67	118.43	126.64
2	A	401	VIR	C23-C22-C20	-4.60	118.94	125.89
3	A	301	COA	O6A-CCP-CBP	4.50	117.78	110.55
2	E	403	VIR	C30-C29-C28	4.19	137.87	126.44
3	D	304	COA	C6P-C5P-N4P	3.92	123.03	116.42
2	A	402	VIR	C4-N5-C6	3.77	124.46	118.83
3	D	304	COA	O5P-C5P-N4P	-3.71	116.00	123.01
2	A	401	VIR	C8-C6-N5	-3.70	113.71	118.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	VIR	C30-C29-C28	3.65	136.40	126.44
2	A	401	VIR	C37-C1-N5	3.40	127.51	123.15
2	E	403	VIR	C30-C32-C33	-3.39	107.64	115.98
2	A	401	VIR	O7-C6-N5	3.38	125.69	120.19
2	A	402	VIR	O36-C32-C33	-3.18	101.83	107.31
2	A	402	VIR	O7-C6-N5	3.16	125.32	120.19
2	A	402	VIR	O15-C14-C13	-3.09	116.15	120.77
2	A	401	VIR	C4-N5-C6	3.03	123.36	118.83
3	D	304	COA	CEP-CBP-CCP	3.02	113.15	108.23
2	A	401	VIR	O38-C37-C1	2.92	131.66	124.19
2	E	403	VIR	O7-C6-N5	2.85	124.82	120.19
3	A	301	COA	C5A-C6A-N6A	2.62	124.34	120.35
3	D	304	COA	C5A-C6A-N6A	2.57	124.27	120.35
3	D	304	COA	C7P-C6P-C5P	-2.55	108.11	112.36
3	E	305	COA	C6P-C7P-N8P	2.53	117.01	111.90
3	E	305	COA	C7P-N8P-C9P	-2.52	118.09	122.59
2	A	401	VIR	C29-C28-C26	-2.50	116.45	122.69
2	A	402	VIR	C16-C17-C19	2.46	115.72	111.10
3	A	301	COA	C7P-C6P-C5P	2.38	116.32	112.36
3	E	305	COA	O6A-CCP-CBP	2.33	114.29	110.55
2	E	403	VIR	C4-N5-C6	2.26	122.21	118.83
3	E	305	COA	CEP-CBP-CCP	2.25	111.91	108.23
2	A	402	VIR	O7-C6-C8	2.23	123.30	119.00
3	A	301	COA	CEP-CBP-CCP	2.18	111.79	108.23
3	D	304	COA	O6A-CCP-CBP	2.18	114.05	110.55
2	E	403	VIR	C23-C22-C20	-2.17	122.61	125.89
2	E	403	VIR	C8-C6-N5	-2.10	115.77	118.48
3	D	304	COA	C2B-C3B-C4B	-2.02	99.65	103.22
3	C	303	COA	C5A-C6A-N6A	2.02	123.42	120.35
3	E	305	COA	C3B-C2B-C1B	2.01	104.35	99.89
2	A	402	VIR	C32-C30-C29	2.01	116.00	109.52
3	E	305	COA	O9P-C9P-N8P	-2.00	118.70	122.99

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	COA	O4B-C4B-C5B-O5B
3	A	301	COA	C5B-O5B-P1A-O1A
3	A	301	COA	CCP-O6A-P2A-O4A
3	A	301	COA	CCP-O6A-P2A-O5A
3	A	301	COA	S1P-C2P-C3P-N4P

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Mol	Chain	Res	Type	Atoms
2	E	403	VIR	C14-C16-C17-O18
2	E	403	VIR	C1-C37-O36-C32
2	A	402	VIR	C14-C16-C17-C19
2	A	402	VIR	C14-C16-C17-O18
2	A	402	VIR	C19-C20-C22-C23
2	A	402	VIR	C21-C20-C22-C23
3	B	302	COA	CCP-O6A-P2A-O4A
3	F	306	COA	C5B-O5B-P1A-O2A
3	F	306	COA	CCP-O6A-P2A-O4A
2	A	401	VIR	C14-C16-C17-O18
3	D	304	COA	C5B-O5B-P1A-O1A
3	D	304	COA	C5B-O5B-P1A-O2A
3	D	304	COA	CCP-O6A-P2A-O4A
3	D	304	COA	CCP-O6A-P2A-O5A
3	D	304	COA	N8P-C9P-CAP-OAP
3	E	305	COA	CCP-O6A-P2A-O4A
2	E	403	VIR	O38-C37-O36-C32
2	E	403	VIR	O27-C26-C28-C29
2	A	402	VIR	O27-C26-C28-C29
2	E	403	VIR	N25-C26-C28-C29
2	A	402	VIR	N25-C26-C28-C29
3	A	301	COA	C3B-C4B-C5B-O5B
3	D	304	COA	O4B-C4B-C5B-O5B
3	C	303	COA	C4B-C3B-O3B-P3B
2	A	402	VIR	C33-C32-O36-C37
3	F	306	COA	O4B-C4B-C5B-O5B
3	D	304	COA	C3B-C4B-C5B-O5B
3	E	305	COA	O4B-C4B-C5B-O5B
3	A	301	COA	C4B-C3B-O3B-P3B
3	B	302	COA	C2B-C3B-O3B-P3B
3	B	302	COA	C4B-C3B-O3B-P3B
3	F	306	COA	C2B-C3B-O3B-P3B
3	F	306	COA	C4B-C3B-O3B-P3B
3	C	303	COA	C2B-C3B-O3B-P3B
3	D	304	COA	C2B-C3B-O3B-P3B
3	D	304	COA	C4B-C3B-O3B-P3B
3	E	305	COA	C2B-C3B-O3B-P3B
3	E	305	COA	C4B-C3B-O3B-P3B
3	A	301	COA	C2B-C3B-O3B-P3B
2	A	402	VIR	C30-C32-O36-C37
3	F	306	COA	C3B-C4B-C5B-O5B
3	E	305	COA	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	E	403	VIR	N5-C1-C37-O38
2	A	402	VIR	N5-C1-C37-O38
2	E	403	VIR	N5-C1-C37-O36
2	A	402	VIR	N5-C1-C37-O36
2	A	402	VIR	C2-C1-C37-O36
3	B	302	COA	O4B-C4B-C5B-O5B
3	D	304	COA	O9P-C9P-CAP-OAP
2	A	402	VIR	C2-C1-C37-O38
2	E	403	VIR	O7-C6-N5-C4
2	A	402	VIR	O7-C6-N5-C4
3	A	301	COA	C5B-O5B-P1A-O3A
2	E	403	VIR	C14-C16-C17-C19
3	B	302	COA	C3B-O3B-P3B-O8A
3	B	302	COA	C5B-O5B-P1A-O3A
3	B	302	COA	CCP-O6A-P2A-O3A
3	F	306	COA	C5B-O5B-P1A-O3A
3	F	306	COA	CCP-O6A-P2A-O3A
3	E	305	COA	C5B-O5B-P1A-O3A
3	E	305	COA	CCP-O6A-P2A-O3A
3	D	304	COA	P2A-O3A-P1A-O1A
3	E	305	COA	P2A-O3A-P1A-O1A
2	A	402	VIR	C31-C30-C32-C33
2	A	401	VIR	C31-C30-C32-C33
2	E	403	VIR	C33-C32-O36-C37
2	A	402	VIR	C31-C30-C32-O36
3	B	302	COA	C5B-O5B-P1A-O1A
3	B	302	COA	CCP-O6A-P2A-O5A
3	F	306	COA	C5B-O5B-P1A-O1A
3	F	306	COA	CCP-O6A-P2A-O5A
2	A	401	VIR	C31-C30-C32-O36
3	E	305	COA	C5B-O5B-P1A-O1A
3	E	305	COA	CCP-O6A-P2A-O5A
2	A	402	VIR	C29-C30-C32-C33
2	A	401	VIR	C29-C30-C32-C33
2	A	402	VIR	C29-C30-C32-O36
2	A	401	VIR	C29-C30-C32-O36
2	A	401	VIR	C8-C6-N5-C1
3	E	305	COA	O9P-C9P-CAP-OAP
3	B	302	COA	C3B-C4B-C5B-O5B
2	A	401	VIR	O7-C6-N5-C4
2	A	402	VIR	O38-C37-O36-C32
3	F	306	COA	S1P-C2P-C3P-N4P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	401	VIR	C28-C29-C30-C31
3	A	301	COA	CCP-O6A-P2A-O3A
3	B	302	COA	C3B-O3B-P3B-O9A
2	A	401	VIR	C14-C16-C17-C19
2	A	401	VIR	O18-C17-C19-C20
3	C	303	COA	CCP-O6A-P2A-O3A
3	D	304	COA	C5B-O5B-P1A-O3A
3	D	304	COA	CCP-O6A-P2A-O3A
2	A	402	VIR	C1-C37-O36-C32
2	E	403	VIR	C8-C6-N5-C1

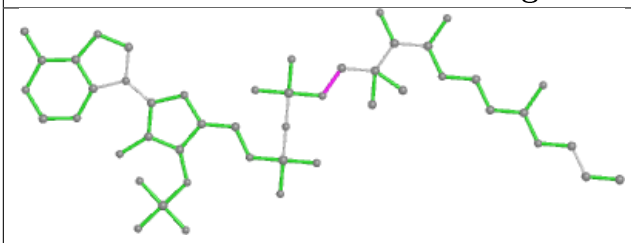
There are no ring outliers.

9 monomers are involved in 53 short contacts:

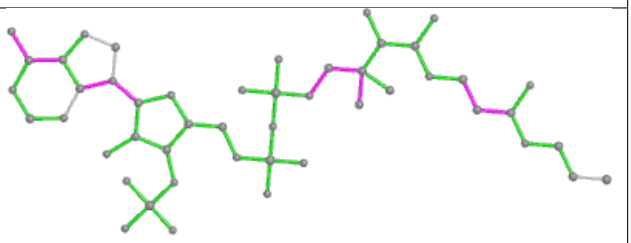
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	COA	4	0
2	E	403	VIR	7	0
2	A	402	VIR	11	0
3	B	302	COA	1	0
3	F	306	COA	2	0
2	A	401	VIR	9	0
3	C	303	COA	8	0
3	D	304	COA	11	0
3	E	305	COA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

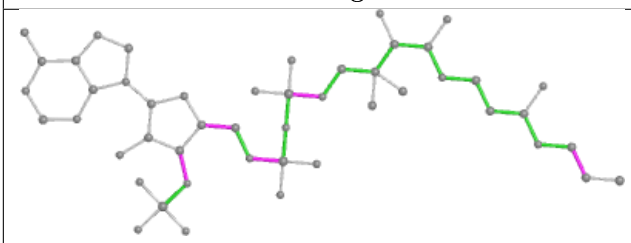
Ligand COA A 301



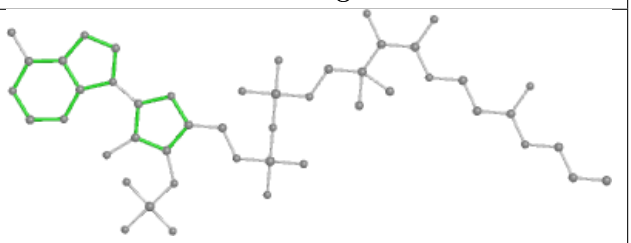
Bond lengths



Bond angles

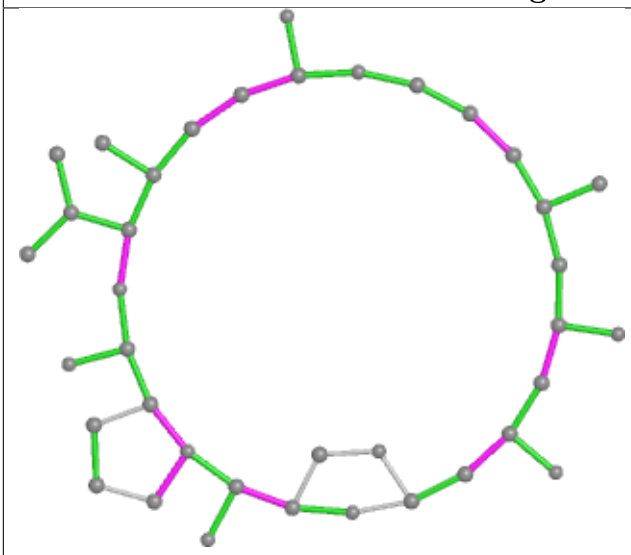


Torsions

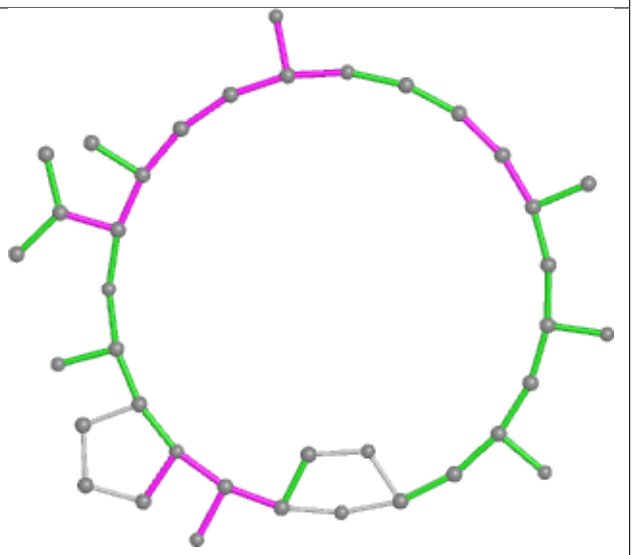


Rings

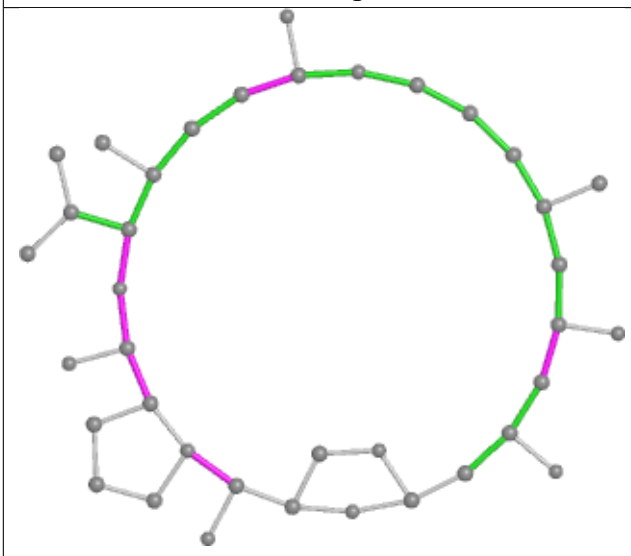
Ligand VIR E 403



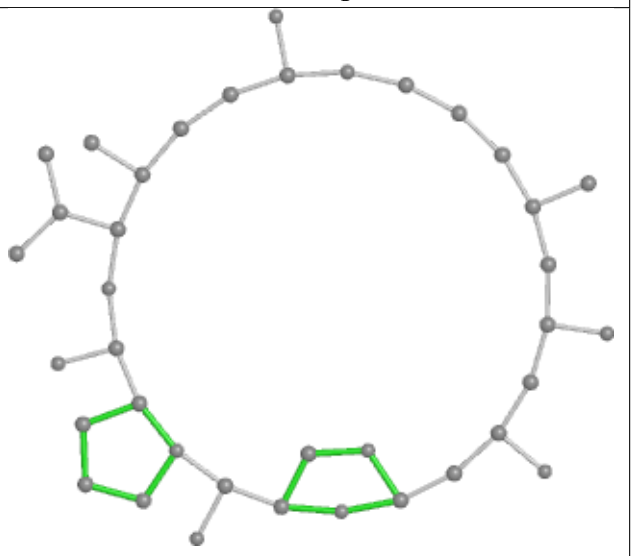
Bond lengths



Bond angles

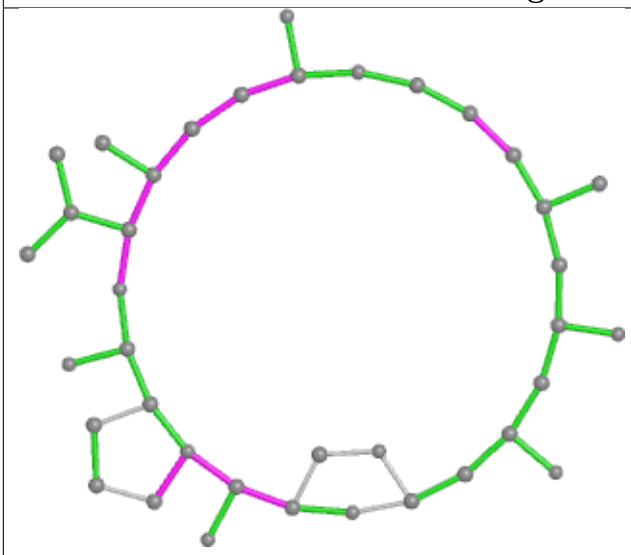


Torsions

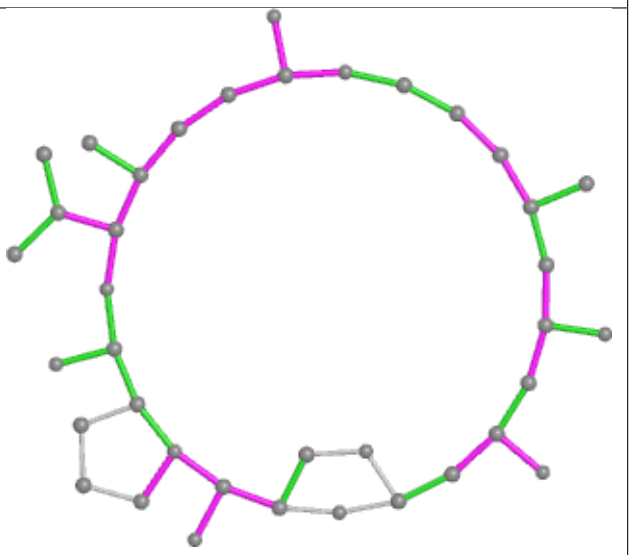


Rings

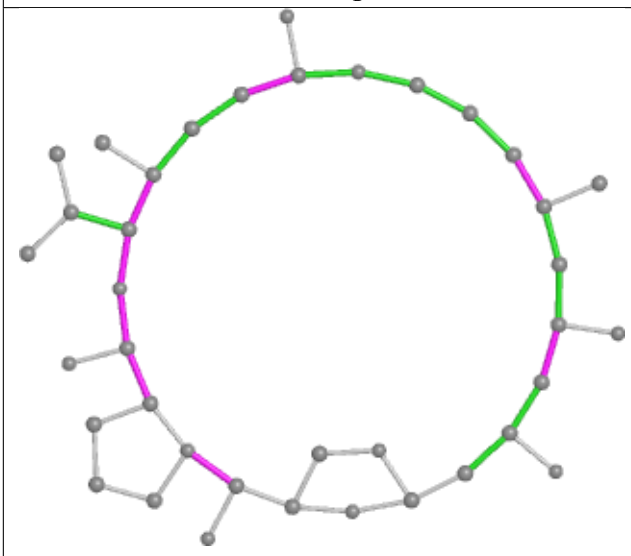
Ligand VIR A 402



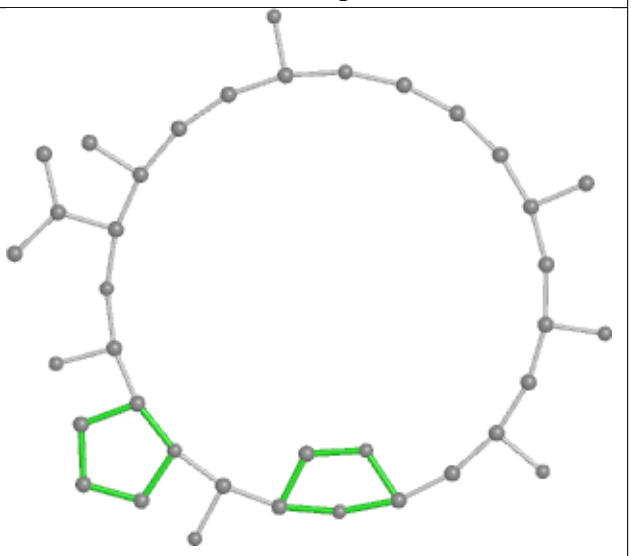
Bond lengths



Bond angles

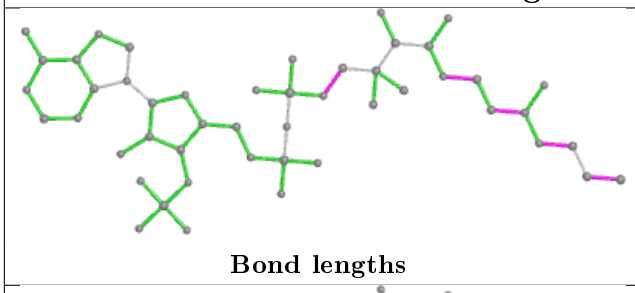


Torsions

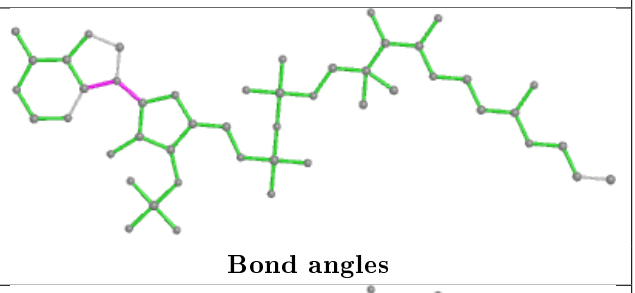


Rings

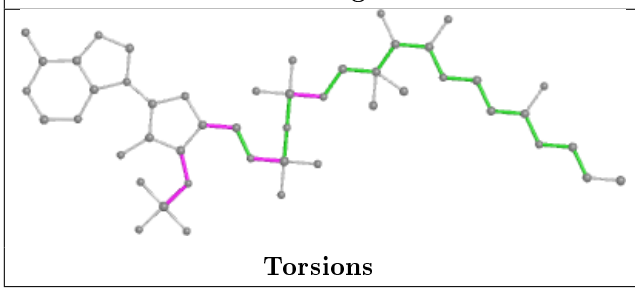
Ligand COA B 302



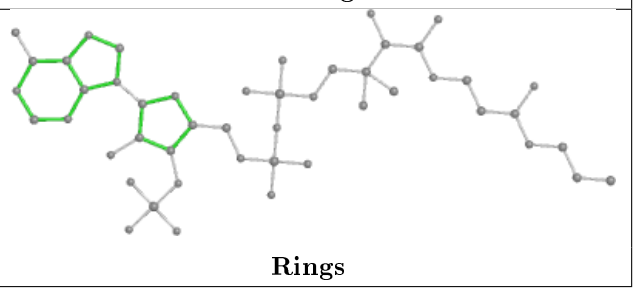
Bond lengths



Bond angles

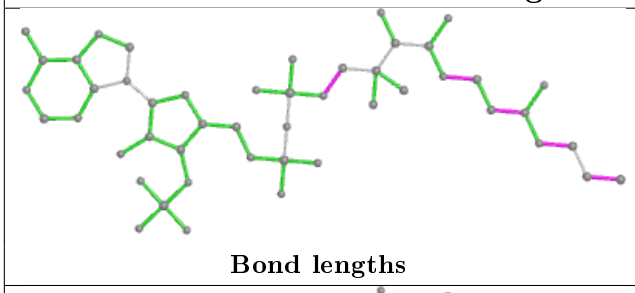


Torsions

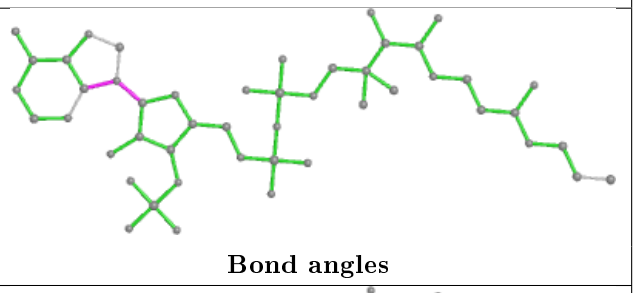


Rings

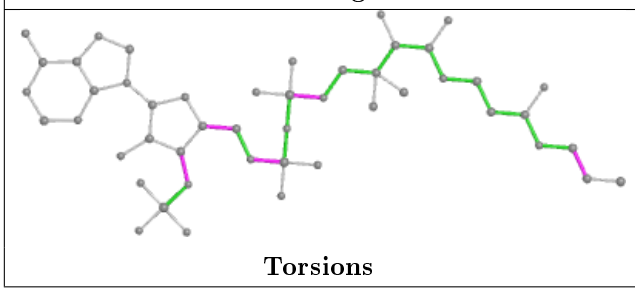
Ligand COA F 306



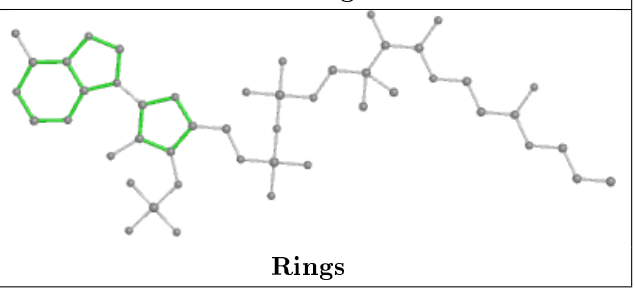
Bond lengths



Bond angles

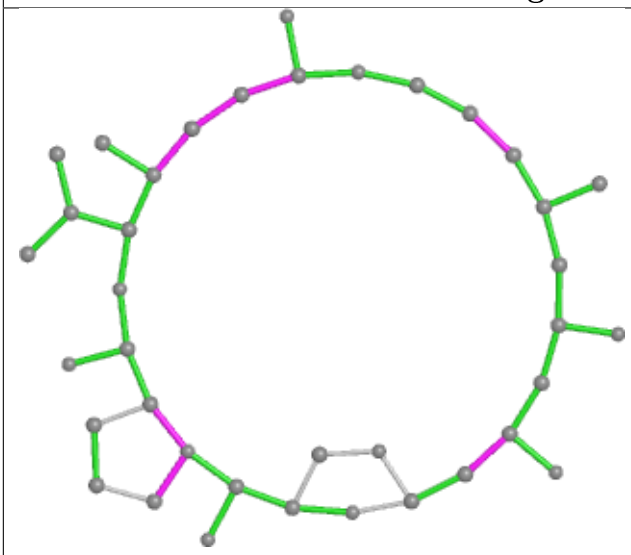


Torsions

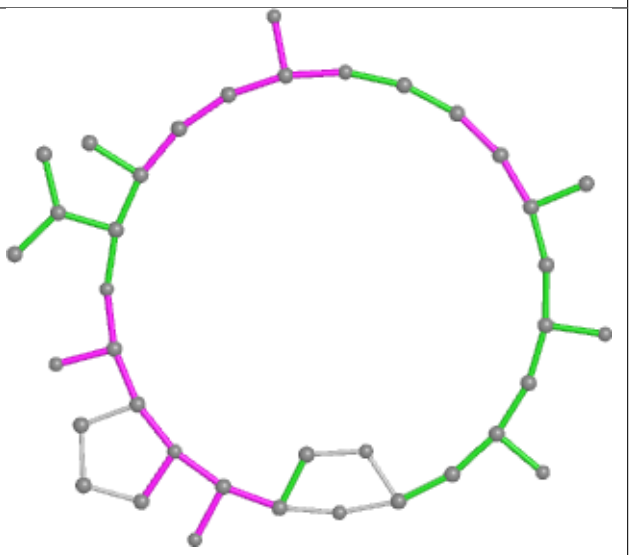


Rings

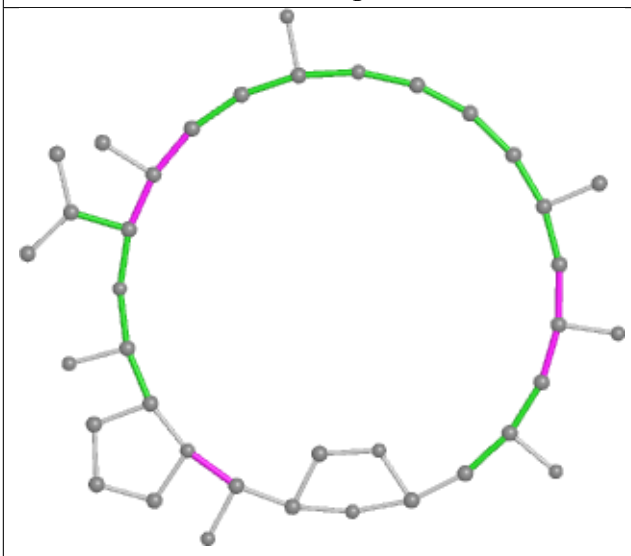
Ligand VIR A 401



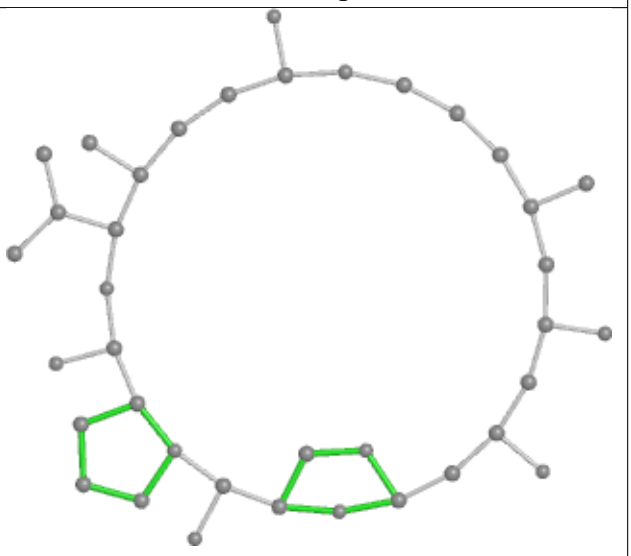
Bond lengths



Bond angles

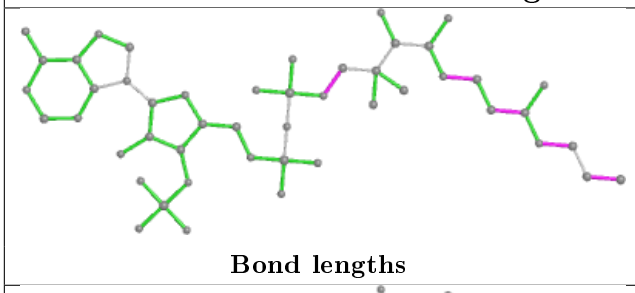


Torsions

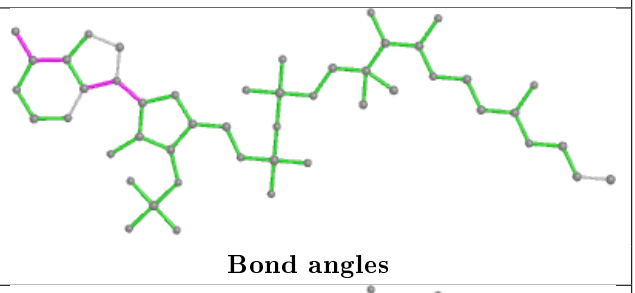


Rings

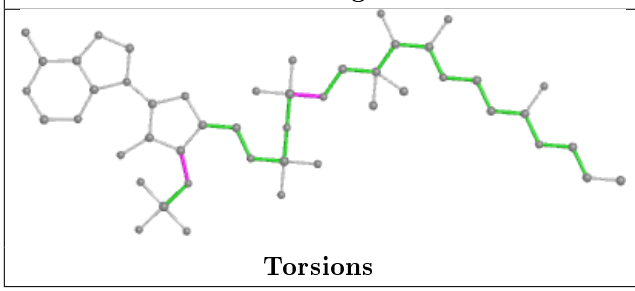
Ligand COA C 303



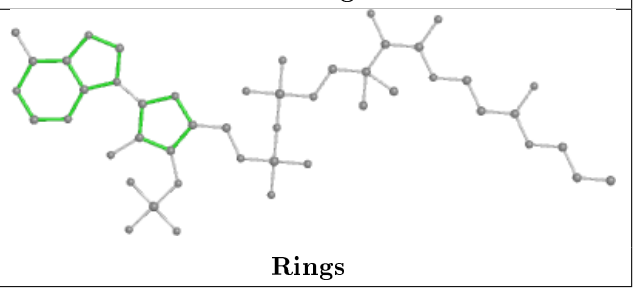
Bond lengths



Bond angles

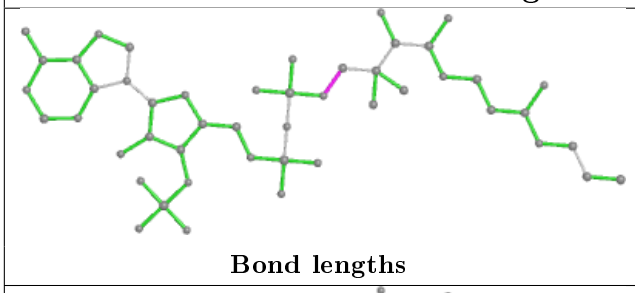


Torsions

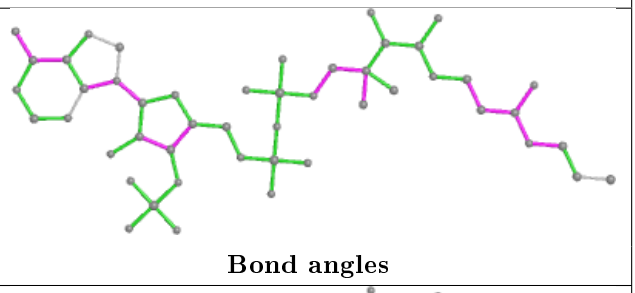


Rings

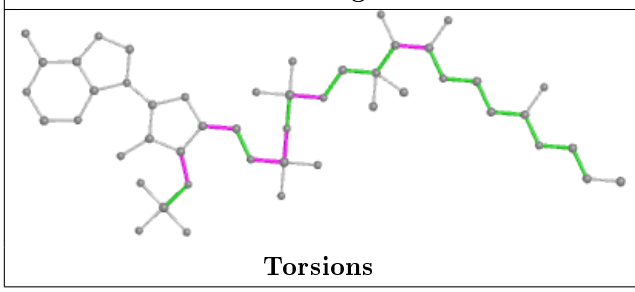
Ligand COA D 304



Bond lengths



Bond angles



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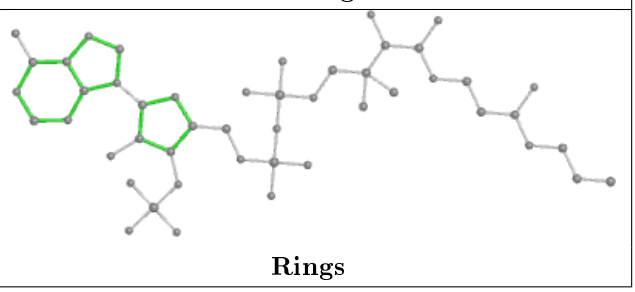
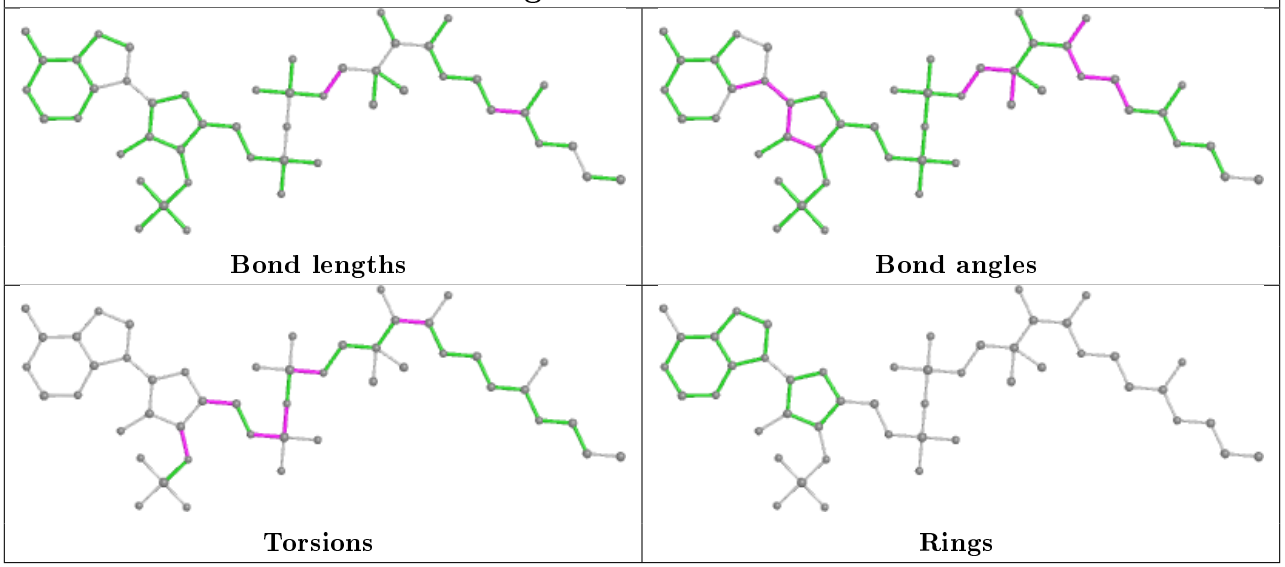


Rings

Ligand COA E 305



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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.