Full wwPDB X-ray Structure Validation Report (i)

Feb 10, 2024 – 08:53 PM EST

PDB ID	:	2II4
Title	:	Crystal structure of a cubic core of the dihydrolipoamide acyltransferase (E2b) component in the branched-chain alpha-ketoacid dehydrogenase complex (BCKDC), Coenzyme A-bound form
Authors	:	Kato, M.; Wynn, R.M.; Chuang, J.L.; Brautigam, C.A.; Custorio, M.; Chuang, D.T.
Deposited on	:	2006-09-27
Resolution	:	2.59 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 (i) 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 (i)) were used in the production of this report:

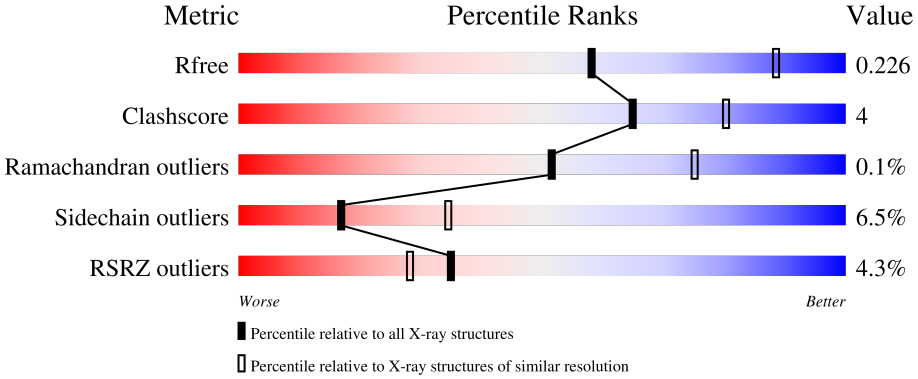
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	262	3% 71% 16% • 11%
1	B	262	2% 74% 13% • 11%
1	C	262	2% 76% 12% • 11%
1	D	262	3% 78% 11% • 11%
1	E	262	3% 77% 11% • 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	262	4% 76% 12% • 11%
1	G	262	8% 77% 11% • 11%
1	H	262	6% 77% 11% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15112 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 Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	234	1803	1158	306	330	9	0	0	0
1	B	234	1803	1158	306	330	9	0	0	0
1	C	234	1803	1158	306	330	9	0	0	0
1	D	234	1803	1158	306	330	9	0	0	0
1	E	234	1803	1158	306	330	9	0	0	0
1	F	234	1803	1158	306	330	9	0	0	0
1	G	234	1803	1158	306	330	9	0	0	0
1	H	234	1803	1158	306	330	9	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	GLY	-	cloning artifact	UNP P11181
A	161	HIS	-	cloning artifact	UNP P11181
B	160	GLY	-	cloning artifact	UNP P11181
B	161	HIS	-	cloning artifact	UNP P11181
C	160	GLY	-	cloning artifact	UNP P11181
C	161	HIS	-	cloning artifact	UNP P11181
D	160	GLY	-	cloning artifact	UNP P11181
D	161	HIS	-	cloning artifact	UNP P11181
E	160	GLY	-	cloning artifact	UNP P11181
E	161	HIS	-	cloning artifact	UNP P11181
F	160	GLY	-	cloning artifact	UNP P11181
F	161	HIS	-	cloning artifact	UNP P11181

Continued on next page...

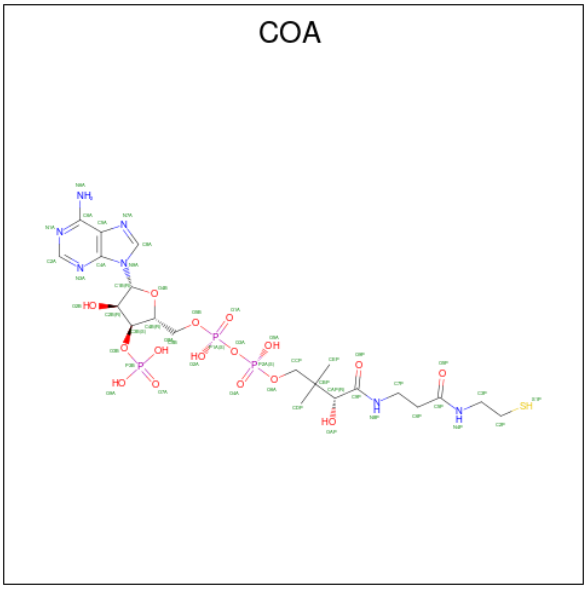
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	160	GLY	-	cloning artifact	UNP P11181
G	161	HIS	-	cloning artifact	UNP P11181
H	160	GLY	-	cloning artifact	UNP P11181
H	161	HIS	-	cloning artifact	UNP P11181

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0
2	G	2	2	2	0	0
2	H	2	2	2	0	0

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

- Molecule 4 is water.

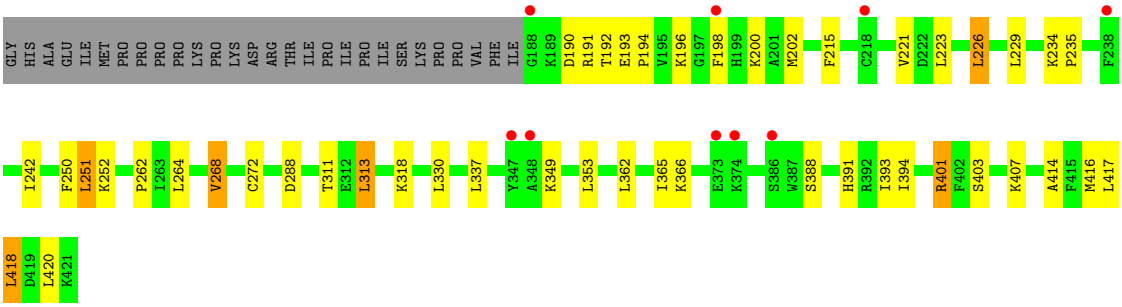
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	46	46	46	0	0
4	B	34	34	34	0	0
4	C	37	37	37	0	0
4	D	33	33	33	0	0
4	E	39	39	39	0	0
4	F	36	36	36	0	0
4	G	26	26	26	0	0
4	H	41	41	41	0	0

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.

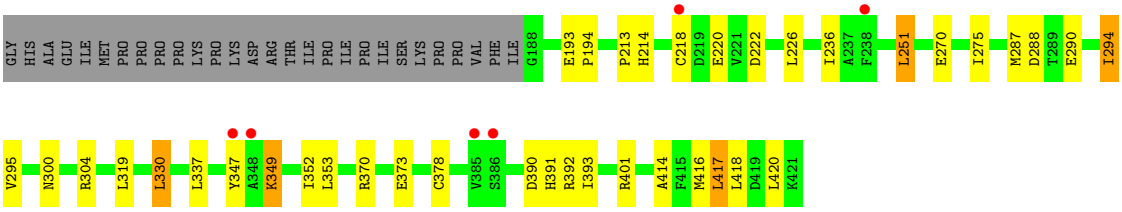
• Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain A:



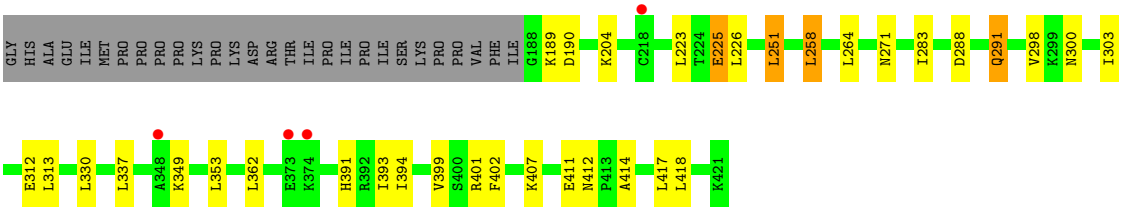
• Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain B:



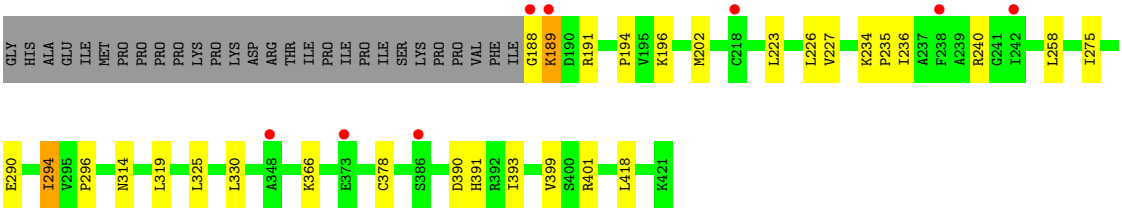
• Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain C:



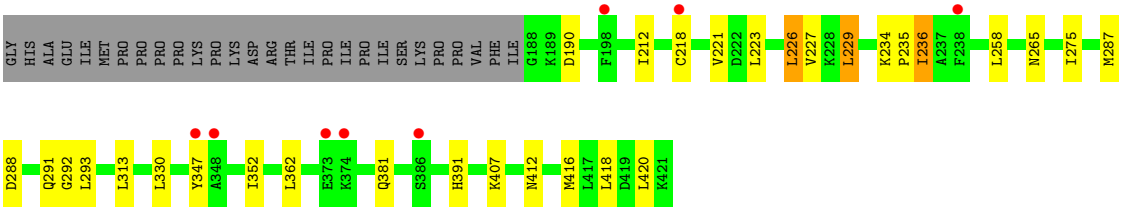
• Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain D:



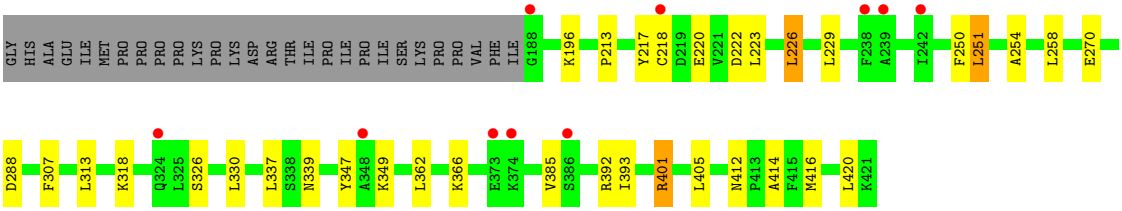
• Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain E:



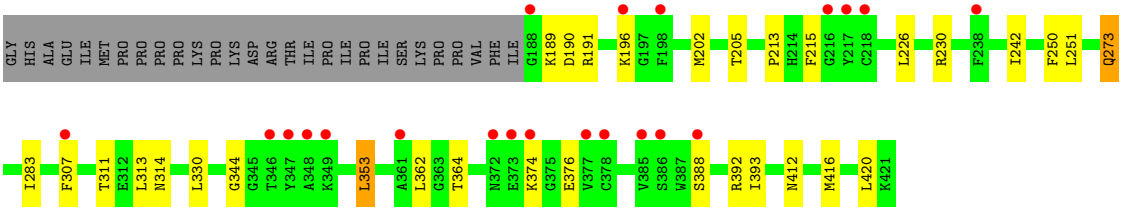
• Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain F:



• Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

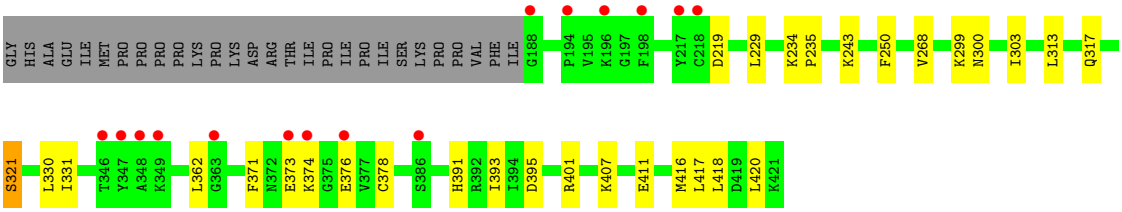
Chain G:



• Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

Chain H:

6%
77%
11%
11%


GLY HIS ALA GLU ILE MET PRO PRO PRO PRO LYS PRO LYS ASP ARG THR ILE PRO ILE PRO ILE SER LYS PRO PRO VAL PHE ILE G188 P194 V195 K196 G197 F198 Y217 C218 D219 L229 K234 P235 K243 F250 V268 K299 N300 I303 L313 Q317
S321 L330 I331 T346 Y347 A348 K349 L362 G363 F371 N372 E373 K374 G375 E376 V377 C378 S386 H391 R392 I393 I394 D395 R401 K407 E411 M416 L417 L418 D419 L420 K421

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	195.23Å 195.23Å 172.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.59 45.26 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.59) 99.8 (45.26-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.94 (at 2.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.229 0.172 , 0.226	Depositor DCC
R_{free} test set	3805 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.008 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15112	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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 (i)

5.1 Standard geometry (i)

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

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	0.94	0/1837	0.88	3/2481 (0.1%)
1	B	0.98	2/1837 (0.1%)	0.92	5/2481 (0.2%)
1	C	0.96	1/1837 (0.1%)	0.90	1/2481 (0.0%)
1	D	0.90	1/1837 (0.1%)	0.89	1/2481 (0.0%)
1	E	0.92	0/1837	0.93	2/2481 (0.1%)
1	F	0.94	2/1837 (0.1%)	0.85	2/2481 (0.1%)
1	G	0.89	0/1837	0.87	1/2481 (0.0%)
1	H	0.96	0/1837	0.90	4/2481 (0.2%)
All	All	0.94	6/14696 (0.0%)	0.89	19/19848 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	270	GLU	CG-CD	6.13	1.61	1.51
1	F	270	GLU	CB-CG	5.73	1.63	1.52
1	C	225	GLU	CG-CD	5.67	1.60	1.51
1	B	378	CYS	CB-SG	-5.59	1.72	1.81
1	D	378	CYS	CB-SG	-5.16	1.73	1.81
1	B	270	GLU	CG-CD	5.06	1.59	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	293	LEU	N-CA-C	-9.46	85.47	111.00
1	G	190	ASP	CB-CG-OD2	6.32	123.98	118.30
1	A	202	MET	CG-SD-CE	6.29	110.26	100.20
1	H	378	CYS	CA-CB-SG	-5.61	103.89	114.00
1	H	401	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	H	395	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	390	ASP	CB-CG-OD1	5.39	123.15	118.30
1	D	390	ASP	CB-CG-OD1	5.32	123.09	118.30
1	H	219	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	190	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	222	ASP	CB-CG-OD1	5.29	123.06	118.30
1	E	190	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	417	LEU	CB-CG-CD1	-5.18	102.19	111.00
1	B	370	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	C	190	ASP	CB-CG-OD1	5.15	122.94	118.30
1	F	401	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	349	LYS	CD-CE-NZ	-5.12	99.92	111.70
1	F	222	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	401	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	291	GLN	Peptide
1	E	292	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1803	0	1859	28	0
1	B	1803	0	1859	17	0
1	C	1803	0	1859	15	0
1	D	1803	0	1859	10	0
1	E	1803	0	1859	15	0
1	F	1803	0	1859	19	0
1	G	1803	0	1859	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1803	0	1859	8	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	48	0	32	2	0
3	B	48	0	32	0	0
3	C	48	0	32	2	0
3	D	48	0	32	1	0
3	E	48	0	32	2	0
3	F	48	0	32	2	0
3	G	48	0	32	2	0
3	H	48	0	32	1	0
4	A	46	0	0	3	0
4	B	34	0	0	0	0
4	C	37	0	0	0	0
4	D	33	0	0	0	0
4	E	39	0	0	1	0
4	F	36	0	0	0	0
4	G	26	0	0	0	0
4	H	41	0	0	0	0
All	All	15112	0	15128	124	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 4.

All (124) 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:B:251:LEU:HD13	1:B:337:LEU:HD12	1.55	0.87
1:A:229:LEU:HD13	1:F:414:ALA:HB1	1.56	0.86
1:C:264:LEU:HD23	1:C:394:ILE:HD13	1.62	0.81
1:E:221:VAL:HG13	1:E:407:LYS:HG3	1.65	0.79
1:C:393:ILE:HG13	1:C:394:ILE:HG13	1.67	0.76
1:E:229:LEU:HD12	1:E:229:LEU:O	1.86	0.76
1:A:229:LEU:CD1	1:F:414:ALA:HB1	2.17	0.74
1:E:234:LYS:HB3	1:E:235:PRO:HD3	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ASP:OD1	1:C:401:ARG:NH2	2.21	0.73
1:C:414:ALA:O	1:C:417:LEU:HB2	1.89	0.73
1:A:264:LEU:HD23	1:A:394:ILE:HD13	1.71	0.72
1:C:251:LEU:HD13	1:C:337:LEU:HD12	1.73	0.70
1:F:223:LEU:HD22	1:F:226:LEU:HD12	1.74	0.68
1:E:288:ASP:OD2	1:F:401:ARG:NH2	2.26	0.68
1:D:401:ARG:NH2	1:F:288:ASP:OD1	2.27	0.68
1:D:188:GLY:O	1:D:189:LYS:HB2	1.94	0.67
1:A:251:LEU:HD13	1:A:337:LEU:HD12	1.76	0.67
1:F:251:LEU:HD13	1:F:337:LEU:HD12	1.77	0.66
1:C:251:LEU:CD1	1:C:337:LEU:HD12	2.27	0.63
1:G:250:PHE:CD2	1:G:362:LEU:HD13	2.33	0.63
1:H:250:PHE:CD2	1:H:362:LEU:HD13	2.34	0.62
1:H:416:MET:O	1:H:420:LEU:HG	2.00	0.62
1:E:229:LEU:HD12	1:E:229:LEU:C	2.22	0.60
1:D:223:LEU:O	1:D:227:VAL:HG23	2.01	0.60
1:A:418:LEU:HD22	1:F:307:PHE:HB2	1.82	0.59
1:A:229:LEU:HD13	1:F:414:ALA:CB	2.29	0.58
1:B:294:ILE:HD13	1:B:295:VAL:H	1.68	0.58
1:E:236:ILE:HD13	1:E:236:ILE:N	2.20	0.57
3:G:500:COA:O4A	3:G:500:COA:H8A	2.05	0.57
1:C:349:LYS:O	1:C:349:LYS:HD3	2.06	0.56
3:E:500:COA:H8A	3:E:500:COA:O4A	2.06	0.56
1:A:223:LEU:HD22	1:A:226:LEU:HD12	1.86	0.56
1:F:251:LEU:CD1	1:F:337:LEU:HD12	2.36	0.55
1:H:317:GLN:O	1:H:321:SER:HB2	2.06	0.55
1:G:205:THR:HG21	1:G:353:LEU:HD12	1.88	0.55
1:A:401:ARG:NH2	1:C:288:ASP:OD1	2.40	0.54
1:E:227:VAL:HG21	1:E:381:GLN:HG3	1.90	0.54
4:A:819:HOH:O	3:C:500:COA:H31	2.08	0.54
1:A:414:ALA:CB	1:F:229:LEU:HD11	2.38	0.53
1:A:192:THR:HG22	1:A:193:GLU:N	2.23	0.53
1:A:414:ALA:HB2	1:F:229:LEU:HD11	1.89	0.53
1:C:407:LYS:O	1:C:411:GLU:HG3	2.09	0.53
3:C:500:COA:O4A	3:C:500:COA:H8A	2.09	0.52
3:F:500:COA:O4A	3:F:500:COA:H8A	2.10	0.52
1:G:374:LYS:HB2	1:G:376:GLU:HG2	1.92	0.52
1:G:242:ILE:HG13	1:G:307:PHE:CE1	2.45	0.52
1:A:288:ASP:OD1	1:B:401:ARG:NH2	2.35	0.52
1:A:268:VAL:HG13	1:A:272:CYS:HA	1.91	0.51
1:A:393:ILE:HG13	1:A:394:ILE:HG13	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:ASN:HB3	4:E:839:HOH:O	2.10	0.50
1:A:349:LYS:O	1:A:349:LYS:HD3	2.12	0.50
1:H:234:LYS:CB	1:H:235:PRO:HD3	2.42	0.49
1:H:407:LYS:O	1:H:411:GLU:HG3	2.12	0.49
1:C:298:VAL:HG13	1:C:312:GLU:HG2	1.95	0.49
1:H:371:PHE:HA	1:H:376:GLU:O	2.12	0.48
1:B:236:ILE:HD12	1:B:236:ILE:H	1.78	0.48
1:D:294:ILE:HG23	1:D:296:PRO:HD3	1.95	0.48
1:D:366:LYS:HB2	1:D:366:LYS:HE3	1.56	0.47
1:G:230:ARG:NH2	3:G:500:COA:O8A	2.31	0.47
3:H:500:COA:H8A	3:H:500:COA:O4A	2.14	0.47
1:F:362:LEU:HD23	1:F:385:VAL:HG23	1.96	0.47
3:A:500:COA:H8A	3:A:500:COA:O4A	2.14	0.47
1:C:300:ASN:HB3	1:C:303:ILE:HG12	1.97	0.46
1:A:416:MET:O	1:A:420:LEU:HG	2.15	0.46
1:E:223:LEU:HD22	1:E:226:LEU:HD12	1.98	0.46
1:D:236:ILE:O	1:D:240:ARG:HG3	2.16	0.46
1:G:416:MET:O	1:G:420:LEU:HG	2.15	0.46
1:F:349:LYS:O	1:F:349:LYS:HD3	2.16	0.46
1:D:234:LYS:N	1:D:235:PRO:HD2	2.29	0.46
1:G:242:ILE:HD12	1:G:311:THR:HA	1.98	0.46
1:B:218:CYS:HB3	1:B:347:TYR:CE1	2.51	0.46
1:F:416:MET:O	1:F:420:LEU:HG	2.16	0.46
1:A:313:LEU:HD13	4:A:839:HOH:O	2.16	0.45
1:G:213:PRO:HG2	1:G:392:ARG:HG3	1.99	0.45
1:G:251:LEU:HD23	1:G:283:ILE:HG21	1.97	0.45
1:B:414:ALA:O	1:B:417:LEU:HB2	2.16	0.45
1:B:287:MET:HG3	1:B:294:ILE:HG22	1.98	0.45
1:E:223:LEU:HA	1:E:223:LEU:HD23	1.62	0.44
1:D:194:PRO:HB2	1:D:196:LYS:HG3	1.98	0.44
1:C:204:LYS:HD3	1:C:204:LYS:HA	1.50	0.44
1:H:300:ASN:HB3	1:H:303:ILE:HG12	2.00	0.44
1:A:250:PHE:CD2	1:A:362:LEU:HD13	2.52	0.44
1:C:258:LEU:HD13	1:C:402:PHE:CE1	2.53	0.44
1:F:213:PRO:HG2	1:F:392:ARG:HG3	2.00	0.43
1:A:251:LEU:CD1	1:A:337:LEU:HD12	2.44	0.43
1:B:294:ILE:HD13	1:B:295:VAL:N	2.33	0.43
3:D:500:COA:H8A	3:D:500:COA:O4A	2.18	0.43
1:A:194:PRO:HG2	1:A:196:LYS:HE2	2.01	0.43
1:E:234:LYS:HB3	1:E:235:PRO:CD	2.42	0.43
1:F:250:PHE:CD2	1:F:362:LEU:HD13	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:273:GLN:HE21	1:G:273:GLN:HB3	1.56	0.43
1:F:254:ALA:O	1:F:258:LEU:HG	2.19	0.43
1:E:416:MET:O	1:E:420:LEU:HG	2.19	0.42
1:F:218:CYS:HB3	1:F:347:TYR:CE1	2.54	0.42
1:G:215:PHE:O	1:G:388:SER:HA	2.19	0.42
1:B:213:PRO:HG2	1:B:392:ARG:HG3	2.02	0.42
1:C:223:LEU:HD23	1:C:223:LEU:HA	1.84	0.42
1:A:234:LYS:N	1:A:235:PRO:HD2	2.35	0.42
1:H:299:LYS:NZ	1:H:331:ILE:O	2.52	0.42
1:A:242:ILE:HD12	1:A:311:THR:HA	2.02	0.42
1:E:218:CYS:HB3	1:E:347:TYR:CE1	2.54	0.42
1:G:344:GLY:HA2	1:G:364:THR:OG1	2.19	0.42
1:A:417:LEU:O	1:A:418:LEU:C	2.58	0.41
1:B:214:HIS:CD2	1:B:352:ILE:HG13	2.55	0.41
1:B:294:ILE:CD1	1:B:330:LEU:HD11	2.50	0.41
1:G:226:LEU:HD12	1:G:226:LEU:HA	1.78	0.41
1:G:251:LEU:CD2	1:G:283:ILE:HG21	2.49	0.41
1:G:273:GLN:H	1:G:273:GLN:HG2	1.76	0.41
1:A:215:PHE:O	1:A:388:SER:HA	2.20	0.41
1:B:275:ILE:HD12	1:B:393:ILE:HD13	2.03	0.41
1:A:403:SER:O	1:A:407:LYS:HB2	2.21	0.41
1:C:251:LEU:HD12	1:C:283:ILE:HG21	2.03	0.41
1:F:339:ASN:HB3	3:F:500:COA:H132	2.03	0.41
1:D:223:LEU:HD23	1:D:223:LEU:HA	1.76	0.41
1:E:212:ILE:HG21	1:E:352:ILE:HD12	2.02	0.41
1:E:287:MET:HB2	3:E:500:COA:H141	2.03	0.41
1:B:300:ASN:O	1:B:304:ARG:HG3	2.21	0.40
1:B:416:MET:O	1:B:420:LEU:HG	2.21	0.40
1:A:252:LYS:HD3	1:A:252:LYS:HA	1.85	0.40
1:B:251:LEU:CD1	1:B:337:LEU:HD12	2.37	0.40
1:A:365:ILE:HG13	3:A:500:COA:N1A	2.37	0.40
1:A:262:PRO:HD2	4:A:817:HOH:O	2.21	0.40
1:D:325:LEU:HD23	1:D:325:LEU:HA	1.94	0.40
1:B:193:GLU:HA	1:B:194:PRO:HD3	1.93	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	232/262 (88%)	225 (97%)	7 (3%)	0	100	100
1	B	232/262 (88%)	223 (96%)	8 (3%)	1 (0%)	34	57
1	C	232/262 (88%)	226 (97%)	6 (3%)	0	100	100
1	D	232/262 (88%)	225 (97%)	6 (3%)	1 (0%)	34	57
1	E	232/262 (88%)	223 (96%)	9 (4%)	0	100	100
1	F	232/262 (88%)	224 (97%)	8 (3%)	0	100	100
1	G	232/262 (88%)	224 (97%)	8 (3%)	0	100	100
1	H	232/262 (88%)	224 (97%)	8 (3%)	0	100	100
All	All	1856/2096 (88%)	1794 (97%)	60 (3%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	189	LYS
1	B	290	GLU

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	196/222 (88%)	182 (93%)	14 (7%)	14	29
1	B	196/222 (88%)	185 (94%)	11 (6%)	21	42
1	C	196/222 (88%)	181 (92%)	15 (8%)	13	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	196/222 (88%)	182 (93%)	14 (7%)	14	29
1	E	196/222 (88%)	184 (94%)	12 (6%)	18	38
1	F	196/222 (88%)	183 (93%)	13 (7%)	16	33
1	G	196/222 (88%)	185 (94%)	11 (6%)	21	42
1	H	196/222 (88%)	184 (94%)	12 (6%)	18	38
All	All	1568/1776 (88%)	1466 (94%)	102 (6%)	17	34

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	ARG
1	A	198	PHE
1	A	200	LYS
1	A	221	VAL
1	A	226	LEU
1	A	251	LEU
1	A	268	VAL
1	A	313	LEU
1	A	318	LYS
1	A	330	LEU
1	A	353	LEU
1	A	366	LYS
1	A	391	HIS
1	A	418	LEU
1	B	220	GLU
1	B	226	LEU
1	B	251	LEU
1	B	294	ILE
1	B	319	LEU
1	B	330	LEU
1	B	349	LYS
1	B	353	LEU
1	B	373	GLU
1	B	391	HIS
1	B	418	LEU
1	C	189	LYS
1	C	225	GLU
1	C	226	LEU
1	C	251	LEU
1	C	258	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	271	ASN
1	C	291	GLN
1	C	313	LEU
1	C	330	LEU
1	C	353	LEU
1	C	362	LEU
1	C	391	HIS
1	C	399	VAL
1	C	412	ASN
1	C	418	LEU
1	D	191	ARG
1	D	202	MET
1	D	226	LEU
1	D	258	LEU
1	D	275	ILE
1	D	290	GLU
1	D	294	ILE
1	D	314	ASN
1	D	319	LEU
1	D	330	LEU
1	D	391	HIS
1	D	393	ILE
1	D	399	VAL
1	D	418	LEU
1	E	226	LEU
1	E	229	LEU
1	E	236	ILE
1	E	258	LEU
1	E	275	ILE
1	E	291	GLN
1	E	313	LEU
1	E	330	LEU
1	E	362	LEU
1	E	391	HIS
1	E	412	ASN
1	E	418	LEU
1	F	196	LYS
1	F	217	TYR
1	F	220	GLU
1	F	226	LEU
1	F	251	LEU
1	F	313	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	318	LYS
1	F	326	SER
1	F	330	LEU
1	F	366	LYS
1	F	393	ILE
1	F	405	LEU
1	F	412	ASN
1	G	189	LYS
1	G	191	ARG
1	G	196	LYS
1	G	202	MET
1	G	273	GLN
1	G	313	LEU
1	G	314	ASN
1	G	330	LEU
1	G	353	LEU
1	G	393	ILE
1	G	412	ASN
1	H	229	LEU
1	H	243	LYS
1	H	268	VAL
1	H	313	LEU
1	H	321	SER
1	H	330	LEU
1	H	373	GLU
1	H	374	LYS
1	H	391	HIS
1	H	393	ILE
1	H	417	LEU
1	H	418	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	A	274	ASN
1	A	328	ASN
1	A	381	GLN
1	B	271	ASN
1	B	291	GLN
1	B	381	GLN
1	C	273	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	274	ASN
1	D	273	GLN
1	D	274	ASN
1	D	324	GLN
1	D	381	GLN
1	E	274	ASN
1	E	381	GLN
1	E	384	ASN
1	F	273	GLN
1	F	274	ASN
1	G	273	GLN
1	G	381	GLN
1	H	273	GLN
1	H	274	ASN
1	H	324	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

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	G	500	-	41,50,50	1.68	3 (7%)	52,75,75	1.71	5 (9%)
3	COA	D	500	-	41,50,50	1.63	3 (7%)	52,75,75	1.39	5 (9%)
3	COA	B	500	-	41,50,50	1.59	3 (7%)	52,75,75	1.54	9 (17%)
3	COA	E	500	-	41,50,50	1.51	3 (7%)	52,75,75	1.64	9 (17%)
3	COA	F	500	-	41,50,50	1.76	3 (7%)	52,75,75	1.26	1 (1%)
3	COA	H	500	-	41,50,50	1.68	3 (7%)	52,75,75	1.65	7 (13%)
3	COA	A	500	-	41,50,50	1.59	3 (7%)	52,75,75	1.40	5 (9%)
3	COA	C	500	-	41,50,50	1.66	3 (7%)	52,75,75	1.36	5 (9%)

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	G	500	-	-	7/44/64/64	0/3/3/3
3	COA	D	500	-	-	3/44/64/64	0/3/3/3
3	COA	B	500	-	-	4/44/64/64	0/3/3/3
3	COA	E	500	-	-	3/44/64/64	0/3/3/3
3	COA	F	500	-	-	5/44/64/64	0/3/3/3
3	COA	H	500	-	-	5/44/64/64	0/3/3/3
3	COA	A	500	-	-	4/44/64/64	0/3/3/3
3	COA	C	500	-	-	7/44/64/64	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	500	COA	O9P-C9P	8.71	1.40	1.23
3	G	500	COA	O9P-C9P	8.64	1.40	1.23
3	H	500	COA	O9P-C9P	8.59	1.40	1.23
3	F	500	COA	O9P-C9P	8.53	1.40	1.23
3	B	500	COA	O9P-C9P	8.23	1.39	1.23
3	C	500	COA	O9P-C9P	7.95	1.39	1.23
3	A	500	COA	O9P-C9P	7.88	1.39	1.23
3	E	500	COA	O9P-C9P	7.08	1.37	1.23
3	F	500	COA	C2A-N3A	4.68	1.39	1.32
3	A	500	COA	C2A-N3A	4.14	1.38	1.32
3	C	500	COA	C2A-N3A	4.09	1.38	1.32
3	G	500	COA	C2A-N3A	4.05	1.38	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	COA	C2A-N3A	3.64	1.38	1.32
3	D	500	COA	C2A-N3A	3.48	1.37	1.32
3	H	500	COA	C2A-N1A	3.45	1.40	1.33
3	E	500	COA	C2A-N3A	3.38	1.37	1.32
3	H	500	COA	C2A-N3A	3.37	1.37	1.32
3	C	500	COA	C2A-N1A	3.22	1.39	1.33
3	F	500	COA	C2A-N1A	3.15	1.39	1.33
3	G	500	COA	C2A-N1A	2.46	1.38	1.33
3	A	500	COA	C2A-N1A	2.44	1.38	1.33
3	D	500	COA	C2A-N1A	2.37	1.38	1.33
3	B	500	COA	C2A-N1A	2.37	1.38	1.33
3	E	500	COA	P3B-O3B	2.02	1.63	1.59

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	500	COA	N3A-C2A-N1A	-7.74	116.58	128.68
3	E	500	COA	N3A-C2A-N1A	-7.16	117.48	128.68
3	B	500	COA	N3A-C2A-N1A	-6.30	118.83	128.68
3	H	500	COA	N3A-C2A-N1A	-5.95	119.37	128.68
3	F	500	COA	N3A-C2A-N1A	-5.89	119.47	128.68
3	D	500	COA	N3A-C2A-N1A	-5.49	120.10	128.68
3	C	500	COA	N3A-C2A-N1A	-5.42	120.21	128.68
3	A	500	COA	N3A-C2A-N1A	-4.72	121.30	128.68
3	A	500	COA	CEP-CBP-CAP	4.38	116.41	108.82
3	D	500	COA	O3B-C3B-C2B	-4.32	96.01	111.68
3	G	500	COA	O3B-C3B-C2B	-4.07	96.93	111.68
3	D	500	COA	CEP-CBP-CAP	4.06	115.86	108.82
3	H	500	COA	CEP-CBP-CAP	3.98	115.72	108.82
3	E	500	COA	O6A-CCP-CBP	-3.82	104.41	110.55
3	G	500	COA	CEP-CBP-CAP	3.73	115.28	108.82
3	C	500	COA	O6A-CCP-CBP	-3.58	104.79	110.55
3	H	500	COA	O3B-C3B-C4B	-3.22	98.43	110.08
3	A	500	COA	O3B-C3B-C2B	-3.07	100.56	111.68
3	B	500	COA	O4B-C4B-C5B	3.06	119.43	109.37
3	H	500	COA	O3B-C3B-C2B	-3.05	100.64	111.68
3	B	500	COA	C5B-C4B-C3B	-3.03	104.34	114.40
3	A	500	COA	C5B-C4B-C3B	-3.02	104.39	114.40
3	E	500	COA	O3B-C3B-C2B	-2.91	101.15	111.68
3	H	500	COA	C6P-C5P-N4P	2.75	121.05	116.42
3	H	500	COA	C7P-N8P-C9P	2.75	127.49	122.59
3	H	500	COA	CEP-CBP-CDP	-2.72	103.62	109.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	500	COA	CEP-CBP-CAP	2.68	113.46	108.82
3	G	500	COA	C2P-C3P-N4P	-2.63	106.29	112.31
3	G	500	COA	O3B-C3B-C4B	-2.62	100.61	110.08
3	E	500	COA	OAP-CAP-CBP	-2.55	104.26	110.25
3	C	500	COA	C5B-C4B-C3B	-2.49	106.14	114.40
3	D	500	COA	C4A-C5A-N7A	-2.41	106.89	109.40
3	E	500	COA	CAP-C9P-N8P	2.37	121.29	116.58
3	B	500	COA	O6A-CCP-CBP	-2.35	106.76	110.55
3	B	500	COA	O9A-P3B-O8A	2.33	116.54	107.64
3	B	500	COA	C3P-N4P-C5P	2.33	127.16	122.84
3	B	500	COA	C6P-C7P-N8P	2.29	116.53	111.90
3	E	500	COA	O9P-C9P-N8P	-2.28	118.09	122.99
3	E	500	COA	O9A-P3B-O8A	2.17	115.94	107.64
3	C	500	COA	CEP-CBP-CAP	2.15	112.56	108.82
3	B	500	COA	C4A-C5A-N7A	-2.14	107.17	109.40
3	C	500	COA	O4B-C4B-C5B	2.14	116.41	109.37
3	D	500	COA	C3B-C2B-C1B	2.14	104.62	99.89
3	E	500	COA	CEP-CBP-CAP	2.08	112.43	108.82
3	E	500	COA	C6P-C7P-N8P	2.08	116.09	111.90
3	A	500	COA	C7P-N8P-C9P	-2.06	118.92	122.59

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	COA	C3B-C4B-C5B-O5B
3	B	500	COA	C3B-C4B-C5B-O5B
3	B	500	COA	O4B-C4B-C5B-O5B
3	C	500	COA	C3B-O3B-P3B-O8A
3	C	500	COA	C3B-C4B-C5B-O5B
3	C	500	COA	O4B-C4B-C5B-O5B
3	D	500	COA	N8P-C9P-CAP-OAP
3	E	500	COA	C5B-O5B-P1A-O1A
3	F	500	COA	C5B-O5B-P1A-O3A
3	G	500	COA	C5B-O5B-P1A-O1A
3	G	500	COA	C5B-O5B-P1A-O2A
3	G	500	COA	N8P-C9P-CAP-OAP
3	H	500	COA	C5B-O5B-P1A-O3A
3	A	500	COA	O4B-C4B-C5B-O5B
3	G	500	COA	C3B-C4B-C5B-O5B
3	G	500	COA	O4B-C4B-C5B-O5B
3	C	500	COA	O9P-C9P-CAP-OAP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	500	COA	O9P-C9P-CAP-OAP
3	F	500	COA	O9P-C9P-CAP-OAP
3	G	500	COA	O9P-C9P-CAP-OAP
3	H	500	COA	P2A-O3A-P1A-O5B
3	A	500	COA	C3B-O3B-P3B-O8A
3	E	500	COA	C5B-O5B-P1A-O3A
3	B	500	COA	C5B-O5B-P1A-O2A
3	C	500	COA	C5B-O5B-P1A-O1A
3	F	500	COA	C5B-O5B-P1A-O2A
3	H	500	COA	C5B-O5B-P1A-O2A
3	F	500	COA	C3B-C4B-C5B-O5B
3	A	500	COA	O9P-C9P-CAP-OAP
3	B	500	COA	O9P-C9P-CAP-OAP
3	E	500	COA	O9P-C9P-CAP-OAP
3	H	500	COA	O9P-C9P-CAP-OAP
3	F	500	COA	O4B-C4B-C5B-O5B
3	C	500	COA	N8P-C9P-CAP-OAP
3	D	500	COA	C3B-O3B-P3B-O7A
3	H	500	COA	N8P-C9P-CAP-OAP
3	C	500	COA	C5B-O5B-P1A-O3A
3	G	500	COA	C5B-O5B-P1A-O3A

There are no ring outliers.

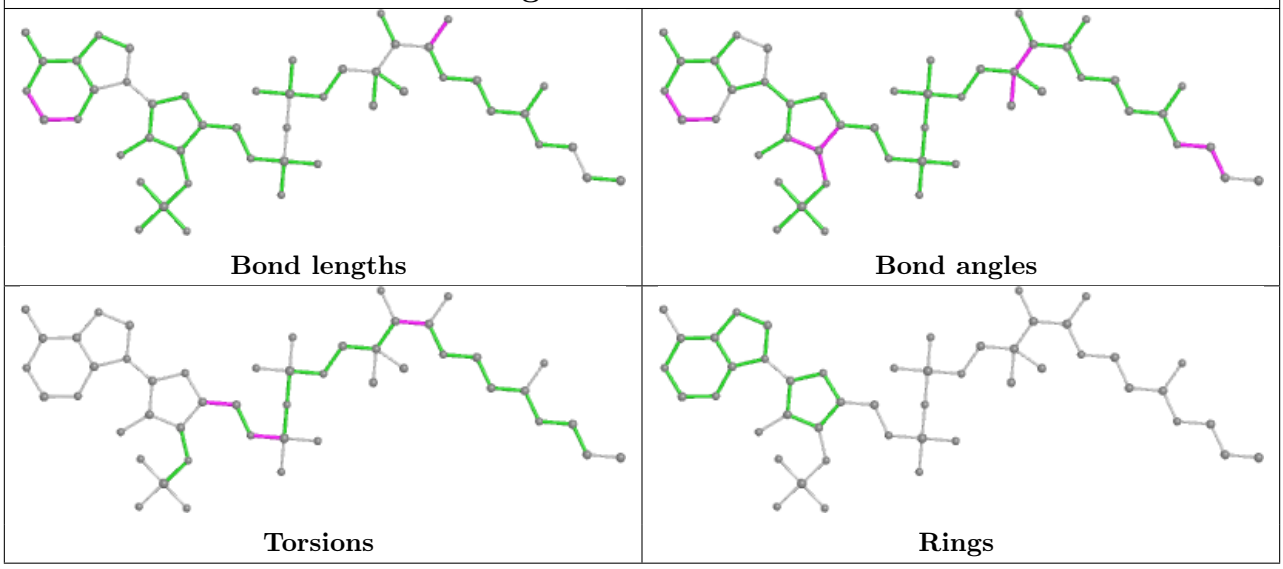
7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	500	COA	2	0
3	D	500	COA	1	0
3	E	500	COA	2	0
3	F	500	COA	2	0
3	H	500	COA	1	0
3	A	500	COA	2	0
3	C	500	COA	2	0

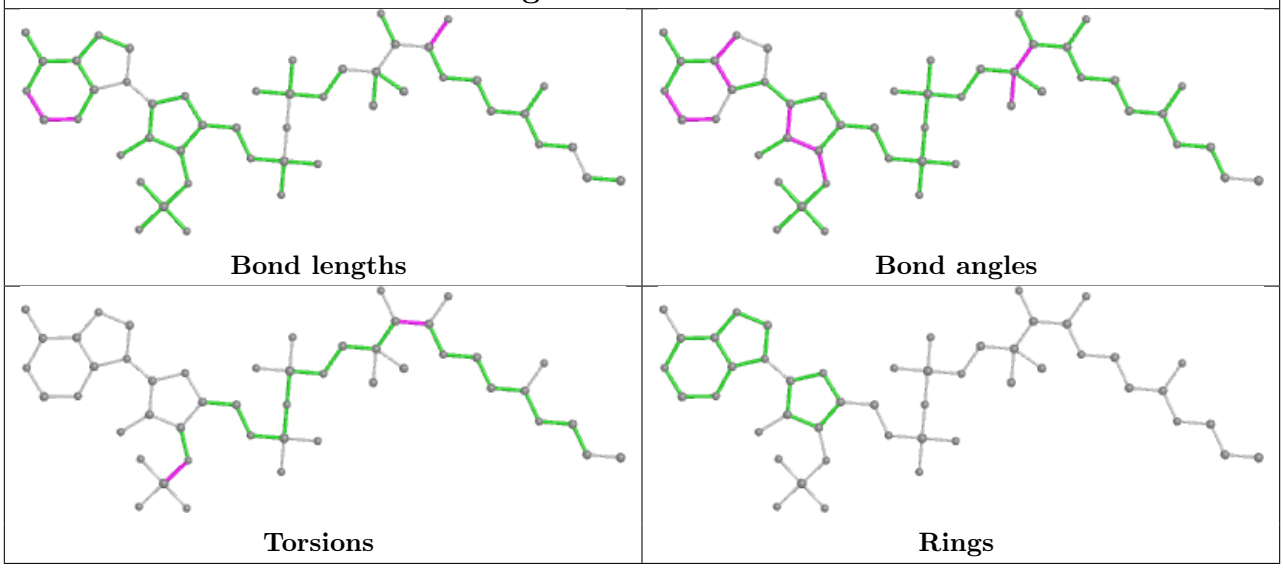
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

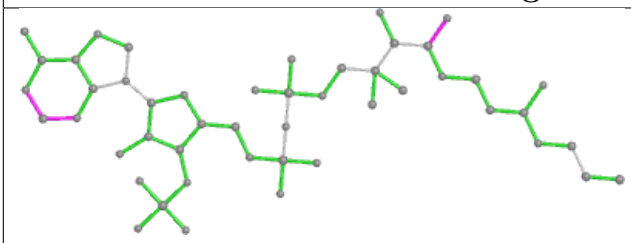
Ligand COA G 500



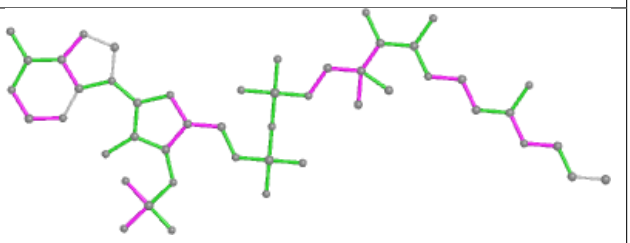
Ligand COA D 500



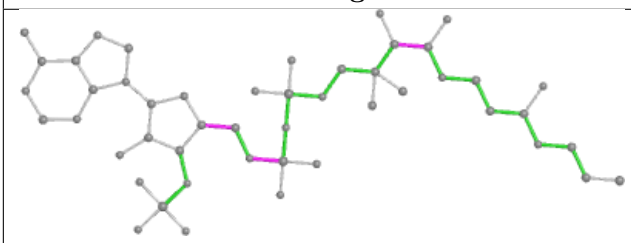
Ligand COA B 500



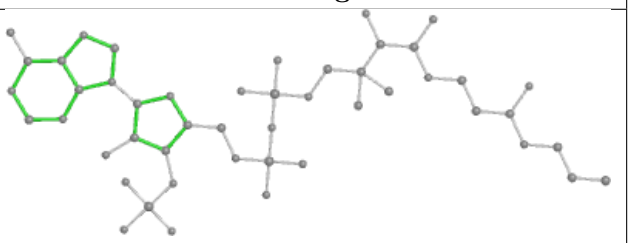
Bond lengths



Bond angles

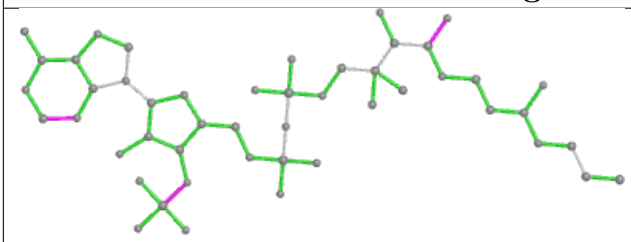


Torsions

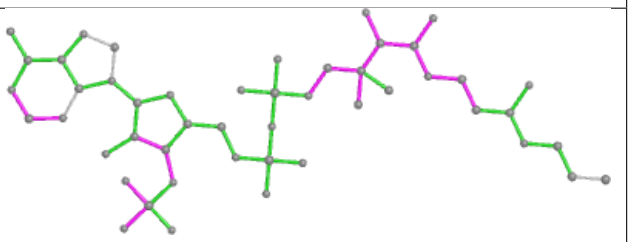


Rings

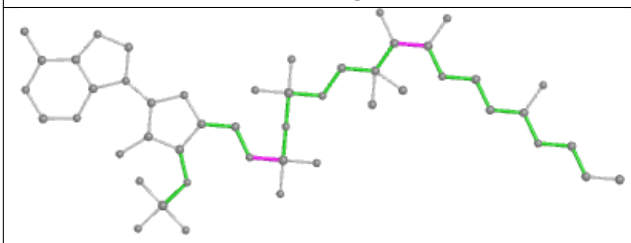
Ligand COA E 500



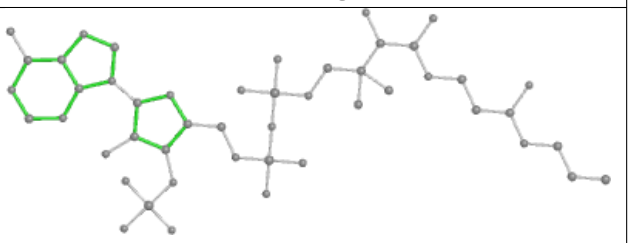
Bond lengths



Bond angles

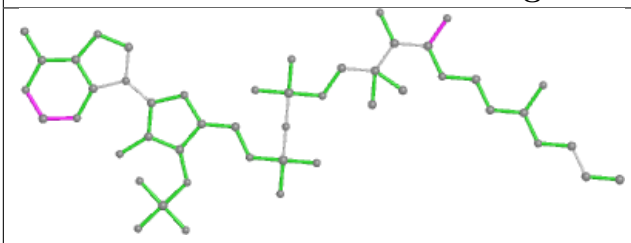


Torsions

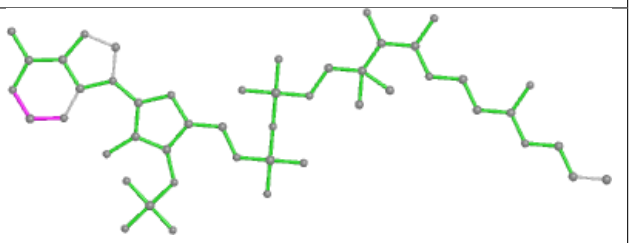


Rings

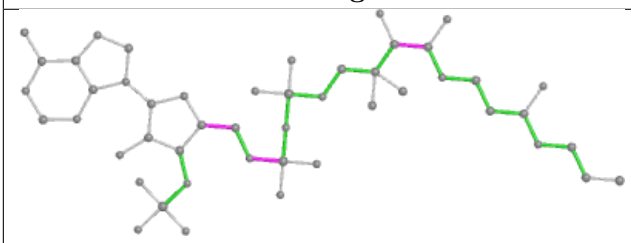
Ligand COA F 500



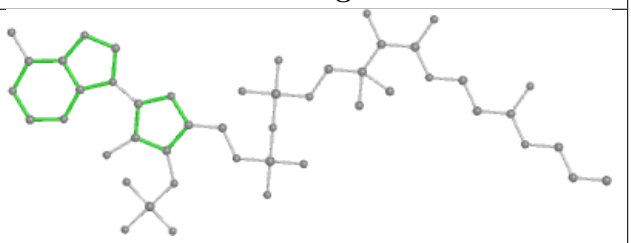
Bond lengths



Bond angles

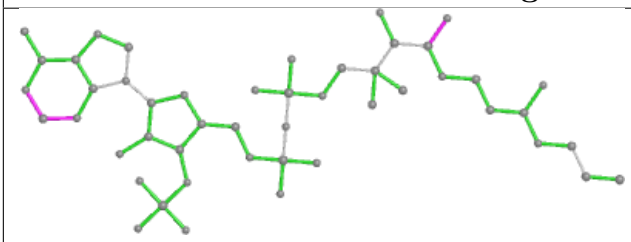


Torsions

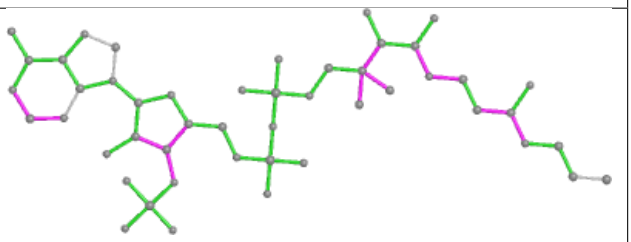


Rings

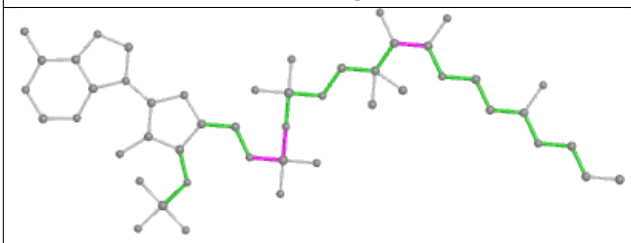
Ligand COA H 500



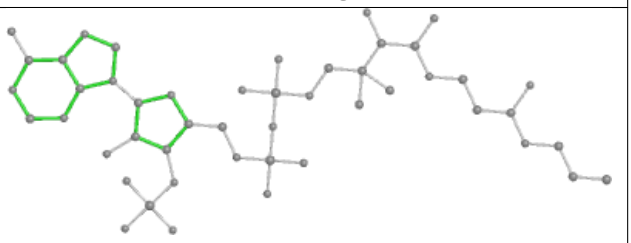
Bond lengths



Bond angles

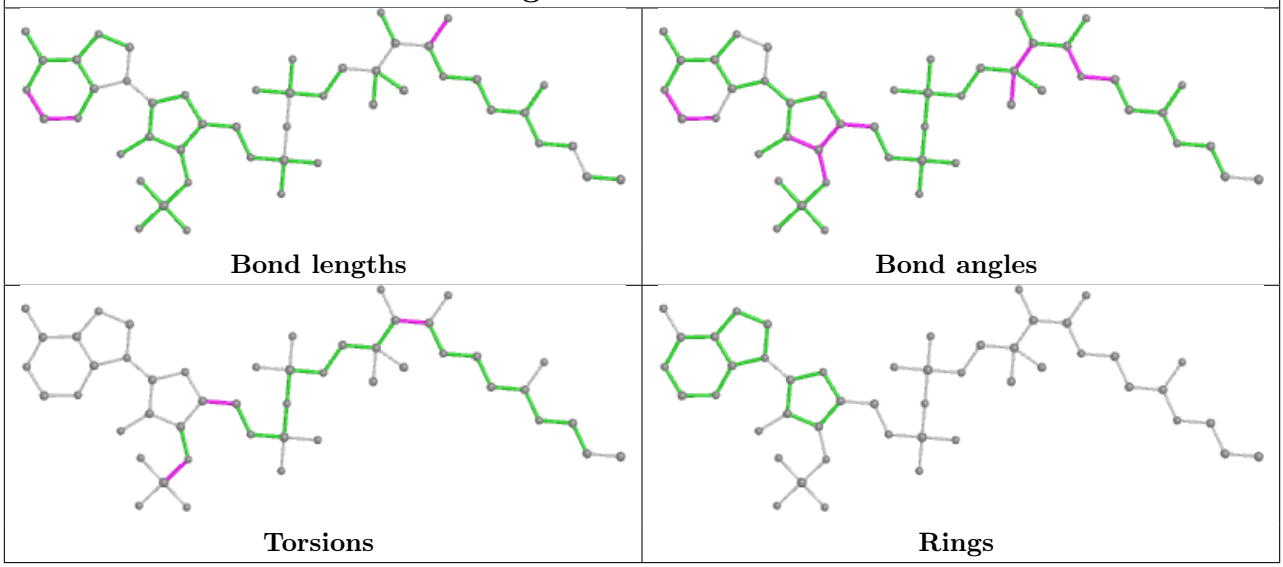


Torsions

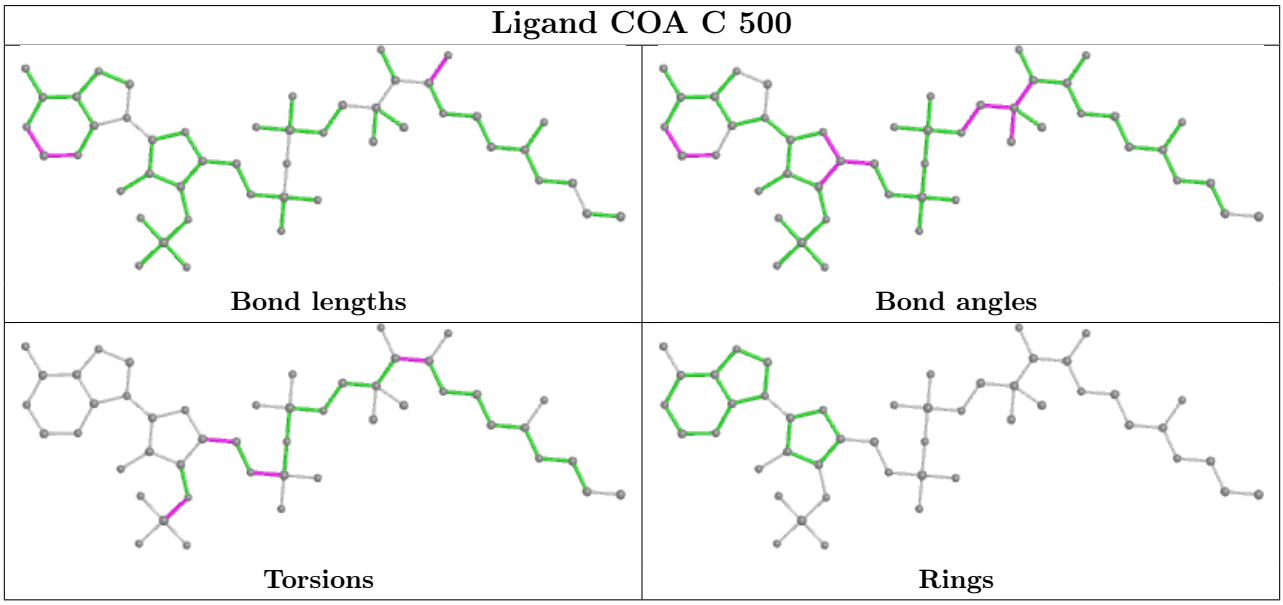


Rings

Ligand COA A 500



Ligand COA C 500



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	234/262 (89%)	-0.11	9 (3%)	40	33	28, 37, 58, 70	0
1	B	234/262 (89%)	-0.07	6 (2%)	56	50	28, 36, 56, 61	0
1	C	234/262 (89%)	-0.10	4 (1%)	70	66	29, 38, 57, 69	0
1	D	234/262 (89%)	-0.00	8 (3%)	45	38	30, 39, 60, 66	0
1	E	234/262 (89%)	-0.06	8 (3%)	45	38	30, 39, 56, 69	0
1	F	234/262 (89%)	0.06	10 (4%)	35	28	30, 40, 58, 64	0
1	G	234/262 (89%)	0.22	21 (8%)	9	6	32, 41, 60, 69	0
1	H	234/262 (89%)	0.09	15 (6%)	19	14	28, 37, 59, 68	0
All	All	1872/2096 (89%)	0.00	81 (4%)	35	28	28, 39, 58, 70	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	188	GLY	4.3
1	H	374	LYS	4.1
1	F	238	PHE	4.0
1	H	218	CYS	3.9
1	H	348	ALA	3.8
1	G	373	GLU	3.8
1	F	188	GLY	3.6
1	G	348	ALA	3.5
1	G	374	LYS	3.5
1	F	218	CYS	3.4
1	H	347	TYR	3.3
1	E	218	CYS	3.3
1	G	347	TYR	3.3
1	G	198	PHE	3.2
1	G	238	PHE	3.2
1	A	188	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	386	SER	3.1
1	E	348	ALA	3.0
1	G	218	CYS	2.9
1	G	377	VAL	2.9
1	D	238	PHE	2.9
1	A	198	PHE	2.8
1	H	196	LYS	2.8
1	H	386	SER	2.8
1	F	374	LYS	2.8
1	D	218	CYS	2.7
1	C	218	CYS	2.7
1	G	349	LYS	2.7
1	D	348	ALA	2.7
1	A	374	LYS	2.7
1	G	188	GLY	2.6
1	H	349	LYS	2.6
1	E	347	TYR	2.6
1	H	217	TYR	2.6
1	G	385	VAL	2.5
1	A	238	PHE	2.5
1	E	198	PHE	2.5
1	A	347	TYR	2.5
1	G	378	CYS	2.5
1	E	374	LYS	2.5
1	B	348	ALA	2.4
1	F	239	ALA	2.4
1	G	216	GLY	2.4
1	G	361	ALA	2.3
1	H	194	PRO	2.3
1	H	373	GLU	2.3
1	H	198	PHE	2.3
1	D	189	LYS	2.3
1	F	348	ALA	2.3
1	F	242	ILE	2.3
1	B	386	SER	2.3
1	E	373	GLU	2.3
1	A	218	CYS	2.3
1	A	373	GLU	2.3
1	F	386	SER	2.2
1	G	217	TYR	2.2
1	H	346	THR	2.2
1	F	324	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	388	SER	2.2
1	B	385	VAL	2.2
1	H	376	GLU	2.2
1	D	242	ILE	2.2
1	C	373	GLU	2.2
1	D	373	GLU	2.2
1	A	386	SER	2.1
1	G	372	ASN	2.1
1	F	373	GLU	2.1
1	B	218	CYS	2.1
1	G	196	LYS	2.1
1	G	346	THR	2.1
1	E	386	SER	2.1
1	A	348	ALA	2.1
1	B	347	TYR	2.1
1	C	348	ALA	2.1
1	C	374	LYS	2.1
1	E	238	PHE	2.1
1	G	307	PHE	2.1
1	H	363	GLY	2.1
1	H	188	GLY	2.0
1	D	386	SER	2.0
1	B	238	PHE	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, 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.

Continued on next page...

Continued from previous page...

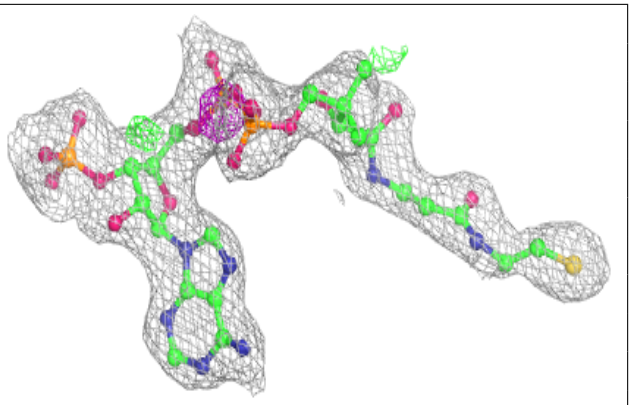
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

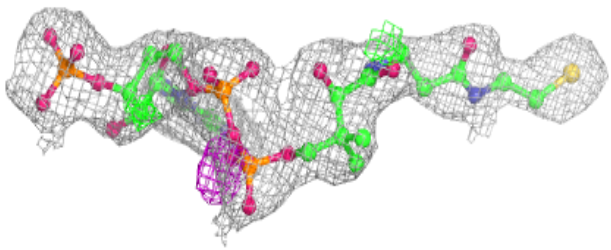
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	B	801	1/1	0.93	0.17	66,66,66,66	0
2	CL	E	806	1/1	0.94	0.34	76,76,76,76	0
2	CL	H	809	1/1	0.94	0.33	65,65,65,65	0
3	COA	D	500	48/48	0.94	0.12	42,52,63,65	0
3	COA	F	500	48/48	0.94	0.13	48,54,63,65	0
2	CL	D	805	1/1	0.95	0.24	71,71,71,71	0
3	COA	C	500	48/48	0.96	0.10	38,43,57,60	0
2	CL	D	808	1/1	0.96	0.10	41,41,41,41	0
3	COA	A	500	48/48	0.96	0.10	34,42,53,55	0
3	COA	G	500	48/48	0.96	0.10	35,43,56,58	0
2	CL	A	802	1/1	0.97	0.24	61,61,61,61	0
3	COA	E	500	48/48	0.97	0.11	31,37,53,57	0
3	COA	B	500	48/48	0.97	0.10	31,42,55,61	0
2	CL	C	803	1/1	0.97	0.25	63,63,63,63	0
3	COA	H	500	48/48	0.97	0.11	32,43,54,58	0
2	CL	C	807	1/1	0.98	0.13	39,39,39,39	0
2	CL	H	812	1/1	0.98	0.11	39,39,39,39	1
2	CL	F	804	1/1	0.98	0.29	71,71,71,71	0
2	CL	G	810	1/1	0.98	0.17	42,42,42,42	1
2	CL	G	811	1/1	0.98	0.40	75,75,75,75	0

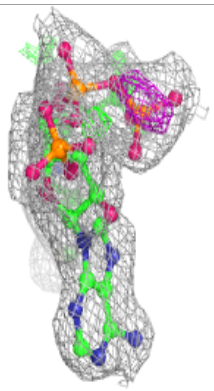
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

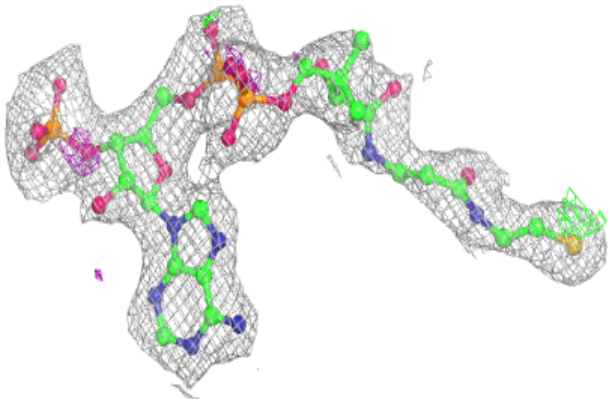


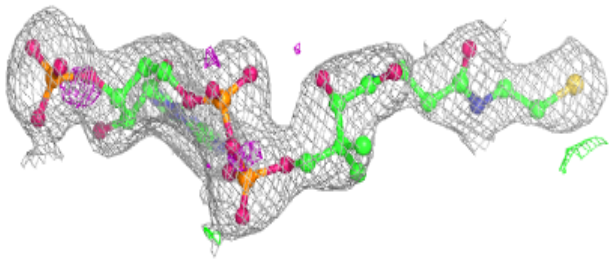


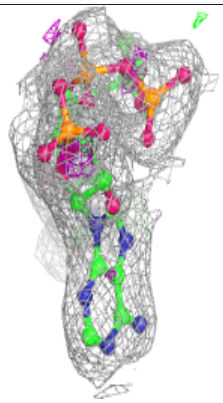


Electron density around COA F 500:

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

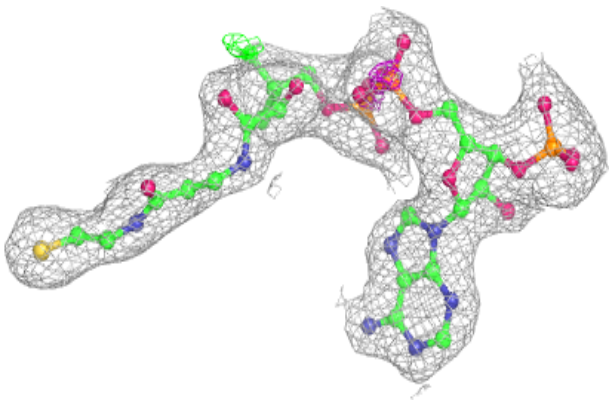


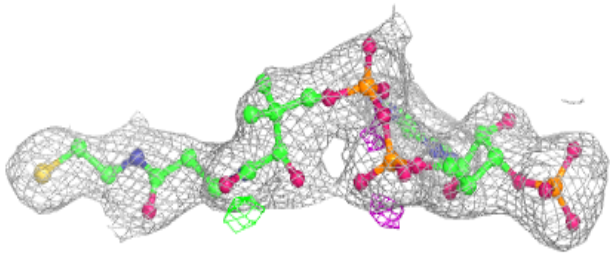


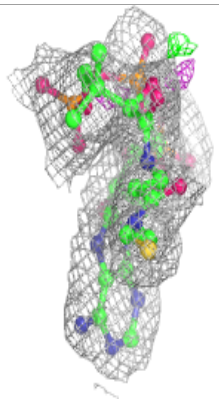


Electron density around COA C 500:

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

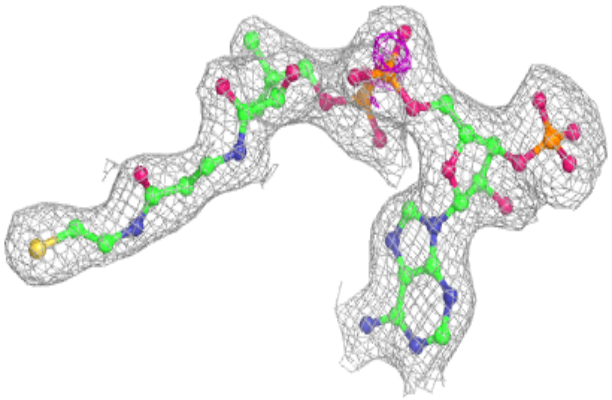


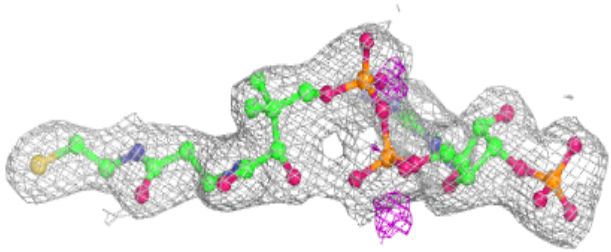


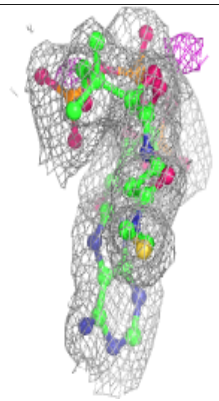


Electron density around COA A 500:

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

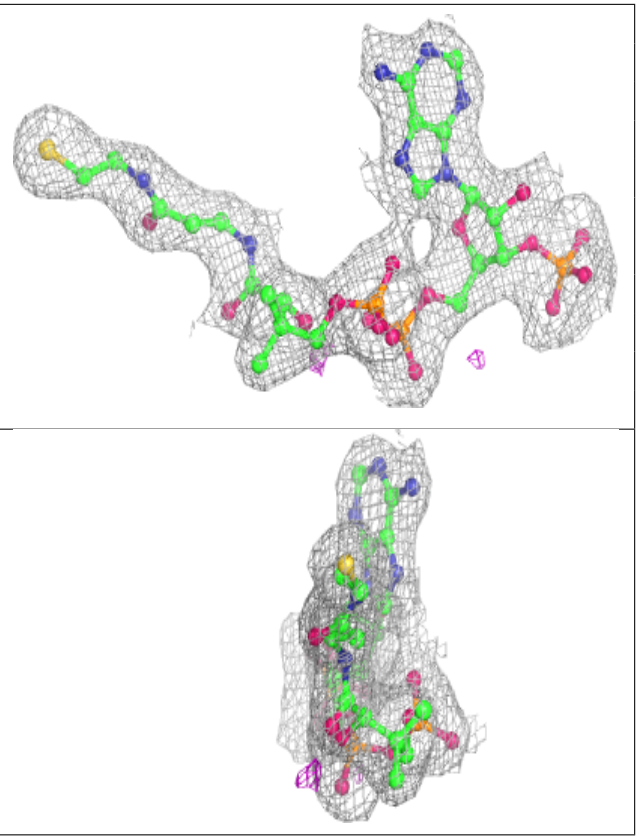


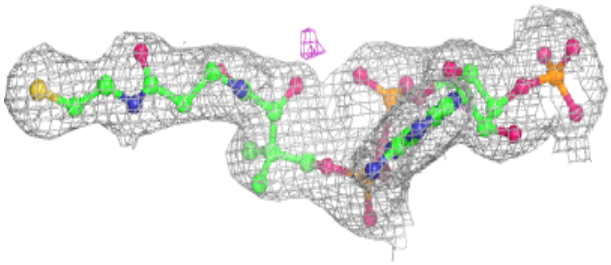




Electron density around COA G 500:

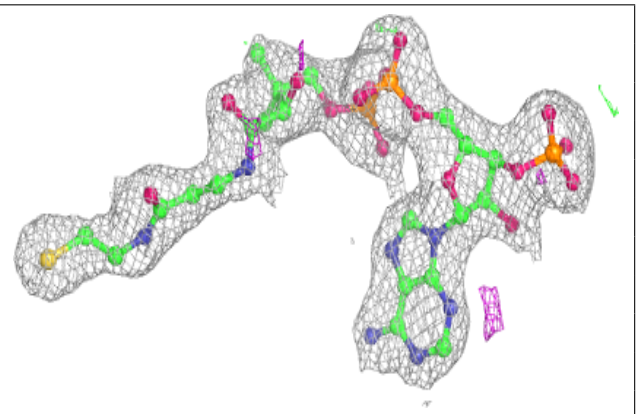
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

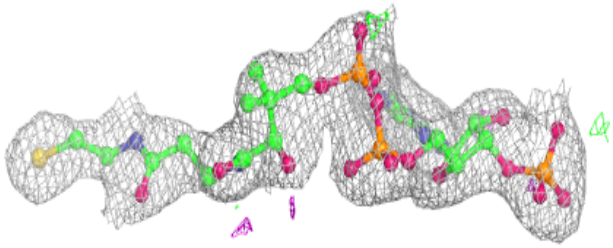


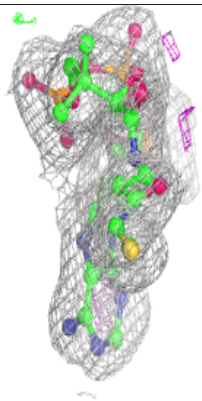


Electron density around COA E 500:

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

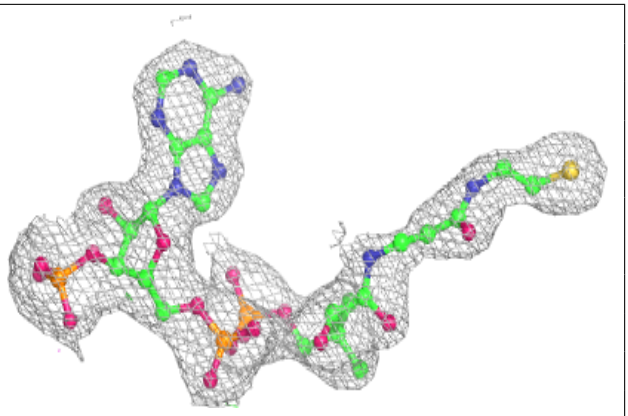


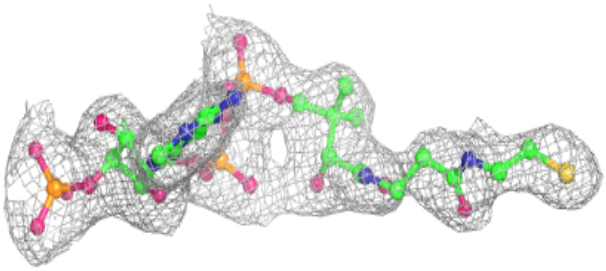


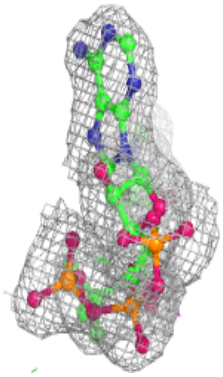


Electron density around COA B 500:

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

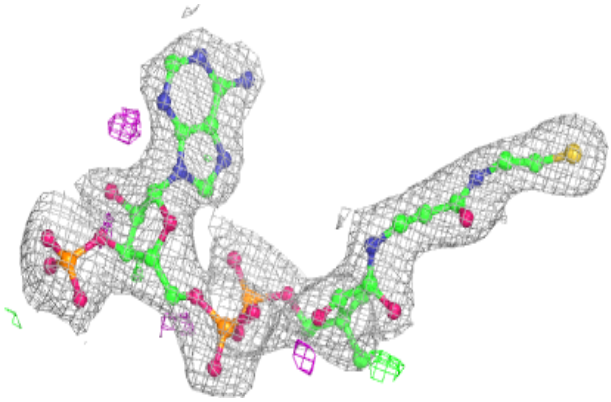


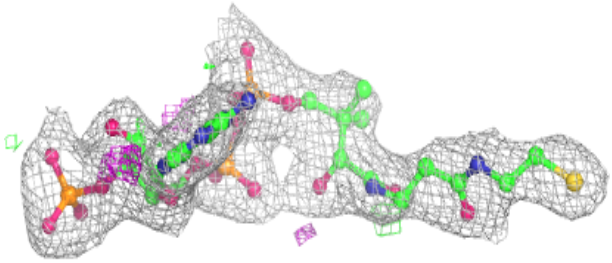


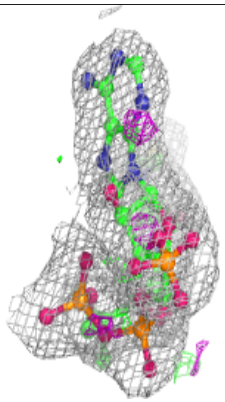


Electron density around COA H 500:

$2mF_o$-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.