



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:11 PM UTC

PDB ID : 2NU7 / pdb_00002nu7
Title : C123aS Mutant of E. coli Succinyl-CoA Synthetase
Authors : Fraser, M.E.
Deposited on : 2006-11-08
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

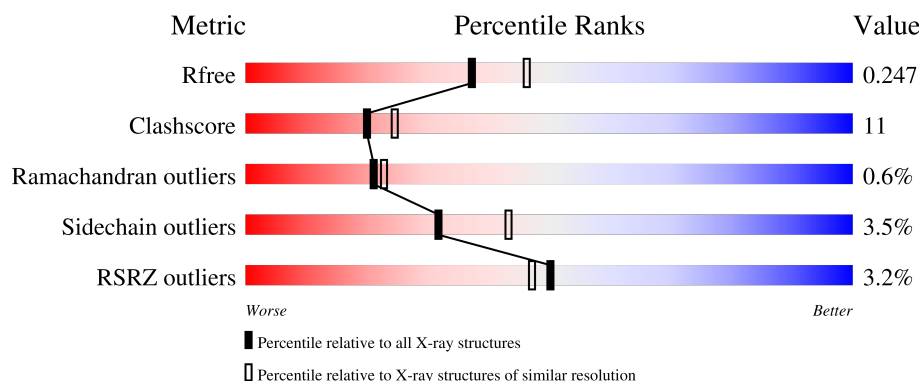
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	288	
1	D	288	
2	B	388	
2	E	388	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	COA	B	1025	-	X	-	-
4	COA	E	1025	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10479 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 Succinyl-CoA ligase [ADP-forming] subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2069	1313	346	400	10			
1	D	287	Total	C	N	O	S	0	0	0
			2069	1313	346	400	10			

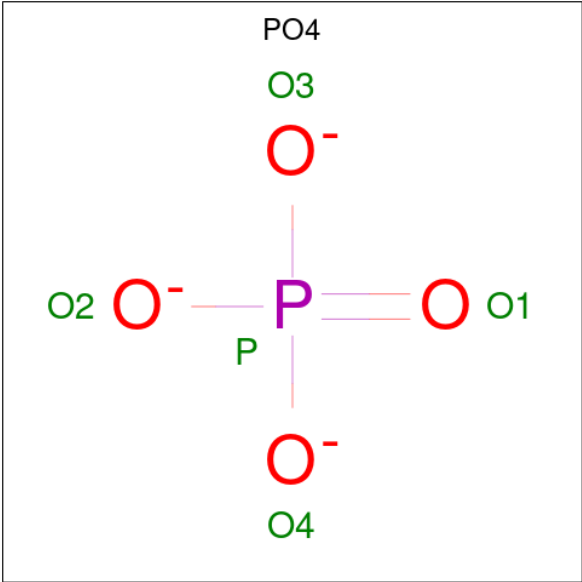
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	SER	CYS	engineered mutation	UNP P0AGE9
D	123	SER	CYS	engineered mutation	UNP P0AGE9

- Molecule 2 is a protein called Succinyl-CoA synthetase beta chain.

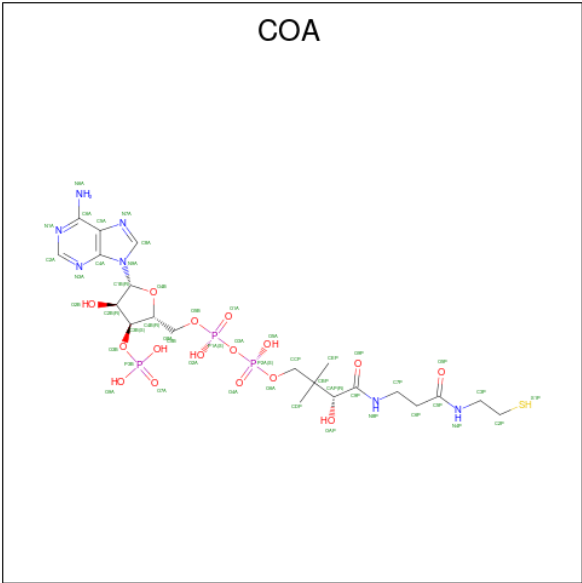
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	388	Total	C	N	O	S	0	0	0
			2908	1836	509	550	13			
2	E	385	Total	C	N	O	S	0	0	0
			2885	1823	505	544	13			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



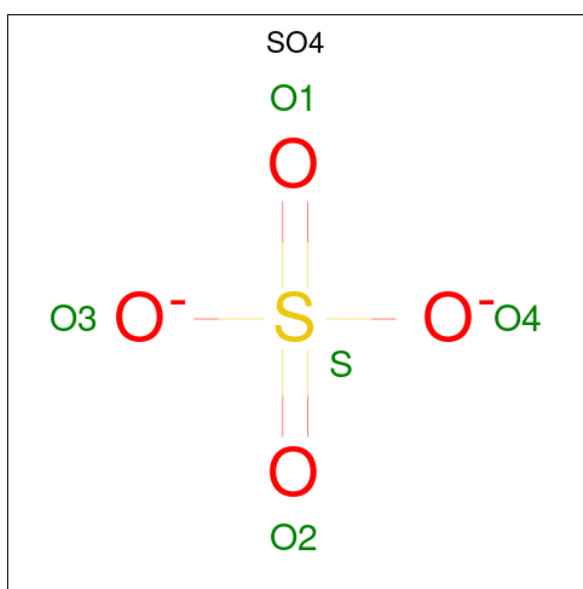
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		
4	B	1	Total	C	N	O S		0	0
			18	11	2	4 1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			18	11	2	4	1		
4	D	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
4	E	1	Total	C	N	O	S	0	0
			18	11	2	4	1		
4	E	1	Total	C	N	O	S	0	0
			9	5	2	1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	101	Total	O	0	0
			101	101		

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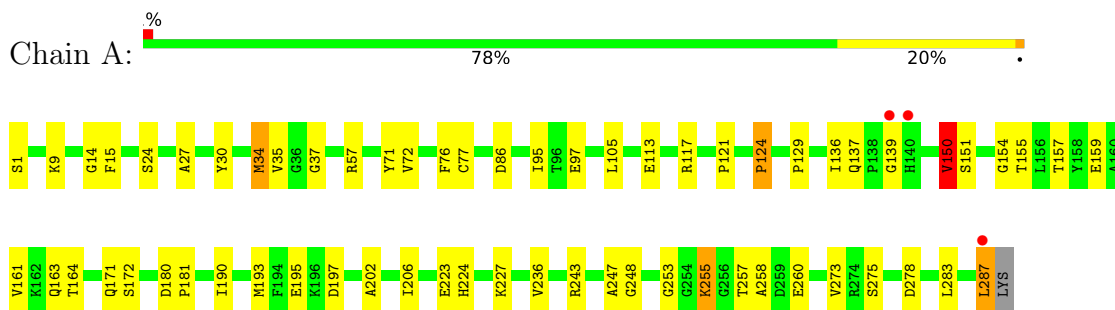
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	103	Total 103	O 103	0	0
6	D	68	Total 68	O 68	0	0
6	E	87	Total 87	O 87	0	0

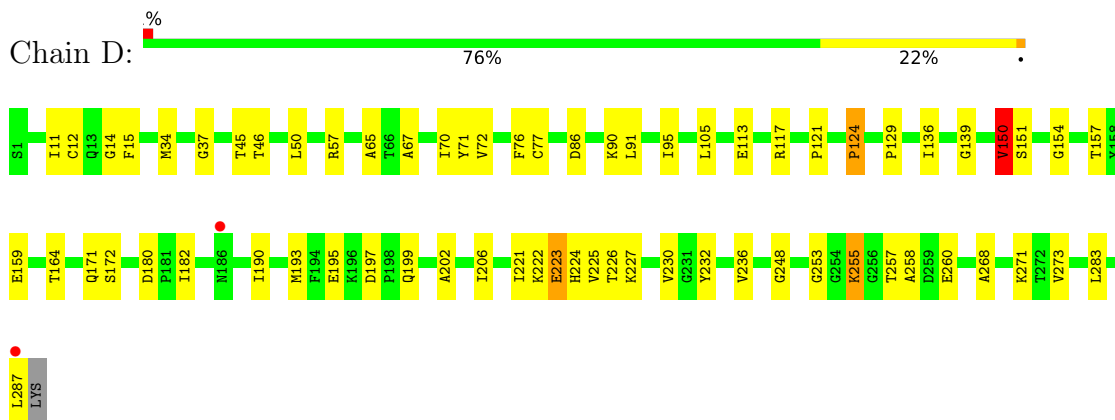
3 Residue-property plots

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.

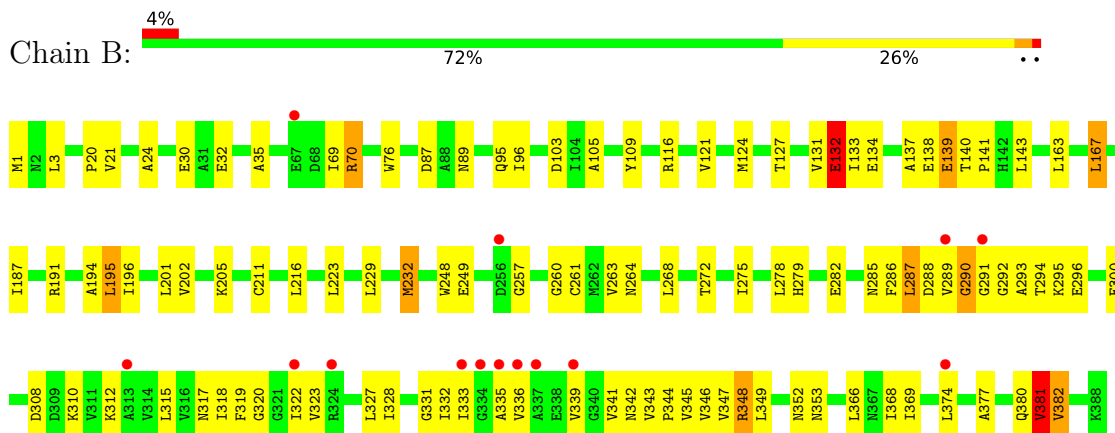
- Molecule 1: Succinyl-CoA ligase [ADP-forming] subunit alpha



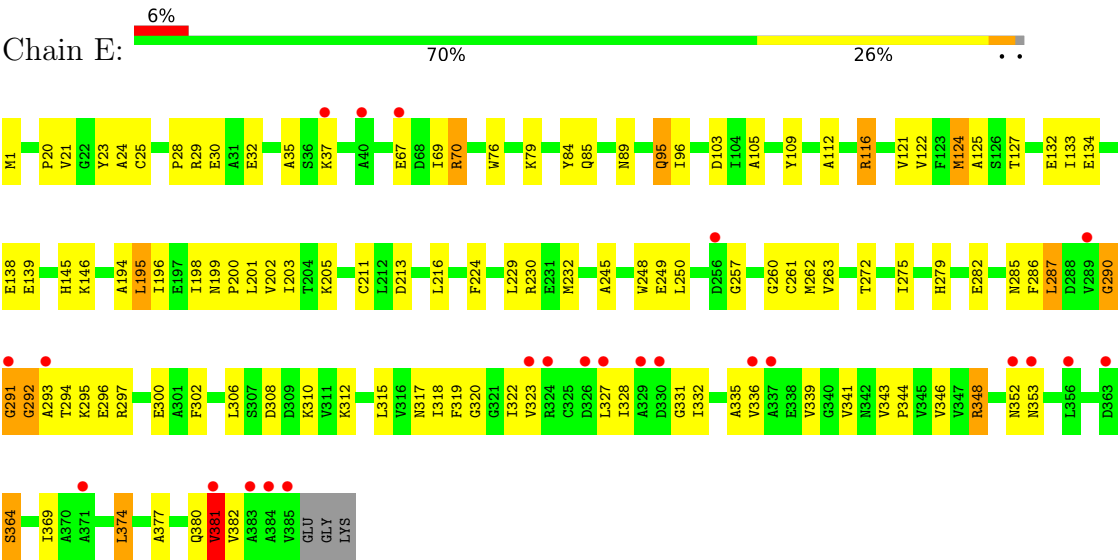
- Molecule 1: Succinyl-CoA ligase [ADP-forming] subunit alpha



- Molecule 2: Succinyl-CoA synthetase beta chain



● Molecule 2: Succinyl-CoA synthetase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	96.63Å 96.63Å 386.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.45 – 2.20 23.45 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.1 (23.45-2.20) 91.1 (23.45-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.15Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.201 , 0.244 0.209 , 0.247	Depositor DCC
R_{free} test set	9773 reflections (11.03%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 24.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10479	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, SO4, PO4

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	0.95	0/2103	1.20	8/2849 (0.3%)
1	D	0.97	2/2103 (0.1%)	1.22	9/2849 (0.3%)
2	B	0.98	2/2950 (0.1%)	1.17	19/3989 (0.5%)
2	E	0.90	0/2927	1.19	19/3961 (0.5%)
All	All	0.95	4/10083 (0.0%)	1.19	55/13648 (0.4%)

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	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	124	MET	SD-CE	7.32	1.97	1.79
2	B	232	MET	SD-CE	-6.13	1.64	1.79
1	D	34	MET	SD-CE	5.42	1.93	1.79
1	D	182	ILE	CA-C	-5.25	1.47	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	LEU	N-CA-C	-9.83	92.71	108.73
2	B	194	ALA	N-CA-C	-9.02	102.43	113.97
2	E	194	ALA	N-CA-C	-8.50	103.43	113.88
2	E	121	VAL	N-CA-C	-8.33	97.90	108.89
2	E	127	THR	N-CA-C	-8.27	103.17	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	139	GLU	N-CA-C	8.23	120.02	111.14
1	D	150	VAL	CB-CA-C	-8.10	98.55	110.62
2	B	201	LEU	N-CA-C	-7.76	94.92	108.20
2	E	364	SER	N-CA-C	7.49	122.41	113.28
1	D	14	GLY	N-CA-C	-7.11	104.80	115.32
1	A	150	VAL	CB-CA-C	-7.05	99.64	110.50
2	B	202	VAL	N-CA-C	6.92	119.03	108.71
2	B	286	PHE	N-CA-C	-6.90	97.96	109.07
1	D	77	CYS	N-CA-C	6.77	118.45	111.14
2	E	203	ILE	N-CA-C	-6.71	98.19	107.99
1	A	77	CYS	N-CA-C	6.69	118.36	111.14
1	A	14	GLY	N-CA-C	-6.66	104.15	115.08
2	E	202	VAL	N-CA-C	6.57	118.51	108.71
1	A	34	MET	N-CA-C	-6.50	100.21	109.96
2	B	343	VAL	CA-C-N	-6.49	113.29	119.85
2	B	343	VAL	C-N-CA	-6.49	113.29	119.85
2	E	139	GLU	N-CA-C	6.41	119.58	111.69
2	E	374	LEU	N-CA-C	6.29	117.93	111.14
1	A	139	GLY	N-CA-C	6.16	121.88	113.99
1	D	34	MET	N-CA-C	-6.09	100.83	109.96
2	E	105	ALA	N-CA-C	-6.05	105.56	113.12
1	D	124	PRO	N-CA-C	-5.99	106.18	114.27
2	B	121	VAL	N-CA-C	-5.99	99.67	108.54
1	D	139	GLY	N-CA-C	5.85	121.48	113.99
2	B	127	THR	N-CA-C	-5.85	106.10	113.18
2	E	21	VAL	N-CA-C	-5.81	102.04	109.30
2	E	286	PHE	N-CA-C	-5.70	99.89	109.07
2	B	105	ALA	N-CA-C	-5.66	106.04	113.12
2	E	76	TRP	N-CA-C	5.51	120.01	113.12
2	E	198	ILE	N-CA-C	-5.46	99.10	106.85
2	B	21	VAL	N-CA-C	-5.44	102.50	109.30
1	D	70	ILE	N-CA-C	5.43	115.67	107.80
2	B	96	ILE	N-CA-C	-5.43	100.51	108.11
2	B	382	VAL	N-CA-C	-5.42	105.21	110.42
1	A	172	SER	N-CA-C	-5.42	102.65	111.04
2	B	76	TRP	N-CA-C	5.41	119.88	113.12
2	B	132	GLU	N-CA-C	-5.40	101.91	109.96
2	E	79	LYS	N-CA-C	-5.40	102.05	110.42
2	E	37	LYS	N-CA-C	-5.38	105.58	111.82
2	B	374	LEU	N-CA-C	5.33	116.89	111.14
1	D	172	SER	N-CA-C	-5.26	102.89	111.04
1	A	24	SER	N-CA-C	-5.24	105.74	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	116	ARG	CB-CG-CD	-5.24	99.25	111.30
2	B	381	VAL	CB-CA-C	-5.22	103.80	112.26
2	E	381	VAL	CB-CA-C	-5.21	103.83	112.26
1	A	124	PRO	N-CA-C	-5.19	107.26	114.27
1	D	45	THR	N-CA-C	-5.13	102.30	109.69
2	E	96	ILE	N-CA-C	-5.11	100.95	108.11
2	B	167	LEU	N-CA-C	-5.11	106.82	113.16
2	B	187	ILE	CB-CA-C	-5.03	105.34	112.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	232	TYR	Sidechain

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	2069	0	2129	49	0
1	D	2069	0	2129	39	0
2	B	2908	0	2961	79	0
2	E	2885	0	2939	76	0
3	A	5	0	0	0	0
3	D	5	0	0	0	0
4	A	48	0	32	3	0
4	B	36	0	40	9	0
4	D	48	0	32	2	0
4	E	27	0	29	8	0
5	B	10	0	0	0	0
5	E	10	0	0	0	0
6	A	101	0	0	2	0
6	B	103	0	0	0	0
6	D	68	0	0	0	0
6	E	87	0	0	4	0
All	All	10479	0	10291	232	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 11.

All (232) 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)
4:B:1325:COA:CBP	4:B:1325:COA:CAP	1.78	1.59
4:B:1025:COA:CAP	4:B:1025:COA:CBP	1.83	1.53
4:E:1025:COA:CBP	4:E:1025:COA:CAP	1.83	1.52
1:D:223:GLU:HG2	1:D:224:HIS:CD2	2.13	0.84
1:A:57:ARG:NH1	1:A:86:ASP:OD2	2.11	0.83
2:B:137:ALA:O	2:B:141:PRO:HG3	1.79	0.83
1:A:223:GLU:HG2	1:A:224:HIS:CD2	2.18	0.78
2:B:336:VAL:HG13	2:B:341:VAL:HB	1.65	0.78
1:D:57:ARG:NH1	1:D:86:ASP:OD2	2.19	0.76
2:B:292:GLY:HA3	2:B:322:ILE:HD11	1.68	0.75
1:D:136:ILE:HD11	4:D:1301:COA:H21	1.70	0.73
2:E:315:LEU:HB2	2:E:381:VAL:HG11	1.70	0.73
2:B:140:THR:HB	2:B:143:LEU:HD12	1.70	0.73
1:A:202:ALA:HB2	1:A:287:LEU:HD11	1.70	0.72
2:B:292:GLY:O	2:B:294:THR:N	2.20	0.71
1:D:257:THR:OG1	1:D:260:GLU:HG3	1.90	0.71
2:B:315:LEU:HB2	2:B:381:VAL:HG11	1.71	0.71
2:E:297:ARG:NH2	6:E:1533:HOH:O	2.23	0.70
2:E:124:MET:HE3	2:E:146:LYS:HE2	1.74	0.69
1:D:202:ALA:HB2	1:D:287:LEU:HD11	1.75	0.69
2:B:195:LEU:HG	2:B:196:ILE:N	2.07	0.68
2:E:32:GLU:OE1	2:E:70:ARG:HD2	1.94	0.68
1:A:136:ILE:HD11	4:A:1300:COA:H21	1.76	0.68
2:E:195:LEU:HG	2:E:196:ILE:N	2.09	0.68
2:E:332:ILE:O	2:E:336:VAL:HG23	1.95	0.66
2:E:318:ILE:HG21	2:E:328:ILE:HD13	1.77	0.66
2:E:346:VAL:HB	2:E:381:VAL:HG13	1.78	0.66
1:D:150:VAL:HG13	1:D:190:ILE:HG21	1.78	0.66
2:B:248:TRP:CD2	2:B:300:GLU:HG3	2.31	0.65
2:B:332:ILE:O	2:B:336:VAL:HG23	1.96	0.65
2:B:229:LEU:HA	2:B:232:MET:HE2	1.77	0.64
2:B:346:VAL:HB	2:B:381:VAL:HG13	1.78	0.64
2:B:248:TRP:CE2	2:B:300:GLU:HG3	2.33	0.64
2:E:312:LYS:O	2:E:343:VAL:HB	1.98	0.64
2:B:140:THR:CB	2:B:143:LEU:HD12	2.29	0.63
2:E:229:LEU:HD23	2:E:232:MET:CE	2.29	0.62
2:B:229:LEU:HD23	2:B:232:MET:CE	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:GLU:OE1	2:B:70:ARG:HD2	2.00	0.62
1:A:257:THR:OG1	1:A:260:GLU:HG3	2.00	0.61
2:E:248:TRP:CD2	2:E:300:GLU:HG3	2.36	0.61
2:E:295:LYS:HG3	2:E:331:GLY:HA2	1.83	0.61
2:E:318:ILE:HG21	2:E:328:ILE:CD1	2.31	0.61
2:B:348:ARG:C	2:B:348:ARG:HD2	2.25	0.61
1:A:150:VAL:HG13	1:A:190:ILE:HG21	1.83	0.60
2:B:289:VAL:O	2:B:291:GLY:N	2.33	0.60
2:E:229:LEU:HA	2:E:232:MET:HE2	1.83	0.60
2:B:318:ILE:HG21	2:B:328:ILE:CD1	2.31	0.60
4:B:1325:COA:CBP	4:B:1325:COA:OAP	2.48	0.60
2:E:248:TRP:CE2	2:E:300:GLU:HG3	2.36	0.60
4:E:1025:COA:CAP	4:E:1025:COA:CCP	2.78	0.59
4:B:1025:COA:CAP	4:B:1025:COA:CCP	2.78	0.59
2:E:260:GLY:HA2	2:E:285:ASN:OD1	2.03	0.58
2:B:292:GLY:O	2:B:294:THR:HG23	2.03	0.58
2:B:336:VAL:HA	2:B:341:VAL:CG2	2.34	0.58
2:E:306:LEU:CD1	2:E:341:VAL:HG22	2.33	0.58
2:E:348:ARG:HD2	2:E:348:ARG:C	2.29	0.58
2:B:260:GLY:HA2	2:B:285:ASN:OD1	2.04	0.57
2:E:312:LYS:O	2:E:344:PRO:HD2	2.04	0.57
2:E:103:ASP:HB3	2:E:205:LYS:HG3	1.87	0.56
1:A:129:PRO:HG2	1:A:171:GLN:HB2	1.87	0.56
2:B:318:ILE:HG21	2:B:328:ILE:HD13	1.88	0.56
1:D:248:GLY:O	2:E:116:ARG:NH2	2.38	0.56
2:E:323:VAL:HG12	2:E:327:LEU:HB2	1.86	0.56
1:A:155:THR:HG21	2:B:264:ASN:O	2.06	0.56
1:D:117:ARG:HD3	1:D:193:MET:HE1	1.88	0.56
1:A:15:PHE:CD2	1:A:37:GLY:HA3	2.41	0.56
2:B:323:VAL:HG12	2:B:327:LEU:HB2	1.86	0.56
2:E:343:VAL:HB	2:E:344:PRO:HD2	1.88	0.56
2:B:295:LYS:HG3	2:B:331:GLY:HA2	1.87	0.55
2:B:139:GLU:C	2:B:141:PRO:HD3	2.31	0.55
2:E:312:LYS:HA	2:E:343:VAL:HG11	1.87	0.55
2:E:230:ARG:HD2	6:E:1562:HOH:O	2.07	0.55
2:B:312:LYS:O	2:B:344:PRO:HD2	2.06	0.55
2:E:124:MET:HA	2:E:145:HIS:O	2.06	0.55
2:E:377:ALA:O	2:E:381:VAL:HG22	2.07	0.55
1:D:15:PHE:CD2	1:D:37:GLY:HA3	2.43	0.54
2:E:292:GLY:O	2:E:294:THR:HG23	2.07	0.54
2:E:292:GLY:HA2	2:E:322:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:PRO:HG2	1:D:171:GLN:HB2	1.89	0.54
1:D:197:ASP:O	1:D:227:LYS:NZ	2.40	0.54
4:E:1025:COA:CBP	4:E:1025:COA:H10	2.20	0.54
2:E:213:ASP:HB3	6:E:1563:HOH:O	2.08	0.54
1:A:253:GLY:O	1:A:255:LYS:HD2	2.07	0.54
2:B:320:GLY:HA2	4:B:1325:COA:H32	1.89	0.54
2:E:35:ALA:HB2	2:E:69:ILE:HD12	1.89	0.53
1:A:197:ASP:O	1:A:227:LYS:NZ	2.42	0.53
2:E:292:GLY:O	2:E:294:THR:N	2.41	0.53
2:E:335:ALA:O	2:E:339:VAL:HB	2.08	0.53
1:D:253:GLY:O	1:D:255:LYS:HD2	2.09	0.53
1:D:253:GLY:HA2	2:E:134:GLU:OE2	2.09	0.53
2:E:369:ILE:HG21	2:E:380:GLN:OE1	2.08	0.53
1:A:181:PRO:O	2:B:116:ARG:HD3	2.10	0.52
2:E:287:LEU:CD1	2:E:287:LEU:C	2.82	0.52
2:B:103:ASP:HB3	2:B:205:LYS:HG3	1.92	0.51
1:A:159:GLU:OE1	2:B:348:ARG:NH2	2.43	0.51
2:E:272:THR:O	2:E:275:ILE:HG22	2.11	0.51
2:E:320:GLY:HA2	4:E:1325:COA:H32	1.93	0.51
2:B:249:GLU:OE2	2:E:70:ARG:NH2	2.43	0.51
1:A:275:SER:HB2	2:B:278:LEU:CD2	2.41	0.50
2:E:229:LEU:HD23	2:E:232:MET:HE2	1.92	0.50
1:D:159:GLU:OE1	2:E:348:ARG:NH2	2.45	0.50
2:E:196:ILE:HG12	2:E:216:LEU:HD22	1.93	0.50
1:A:223:GLU:O	1:A:223:GLU:HG3	2.11	0.50
2:B:377:ALA:O	2:B:381:VAL:HG22	2.12	0.49
1:A:137:GLN:H	1:A:137:GLN:CD	2.20	0.49
2:E:352:ASN:O	2:E:353:ASN:HB2	2.11	0.49
1:A:163:GLN:HG3	6:A:1650:HOH:O	2.12	0.49
2:B:287:LEU:CD1	2:B:287:LEU:C	2.86	0.49
2:B:35:ALA:HB2	2:B:69:ILE:HD12	1.93	0.49
1:D:105:LEU:C	1:D:105:LEU:HD23	2.38	0.49
1:A:151:SER:HB2	1:A:206:ILE:HB	1.94	0.49
1:A:155:THR:HB	2:B:268:LEU:HB2	1.94	0.49
2:B:3:LEU:HD12	2:B:216:LEU:HB2	1.95	0.49
2:B:70:ARG:NH2	2:E:249:GLU:OE2	2.45	0.49
2:E:24:ALA:O	4:E:1025:COA:H21	2.13	0.49
2:E:308:ASP:OD1	2:E:310:LYS:HG2	2.13	0.48
4:B:1325:COA:CAP	4:B:1325:COA:CDP	2.84	0.48
1:D:151:SER:HB2	1:D:206:ILE:HB	1.95	0.48
1:A:236:VAL:HA	1:A:258:ALA:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:VAL:HA	1:D:258:ALA:HB3	1.95	0.48
1:D:164:THR:HG22	1:D:283:LEU:CD1	2.44	0.48
2:E:336:VAL:HG13	2:E:341:VAL:HB	1.95	0.48
1:A:164:THR:HG22	1:A:283:LEU:CD1	2.43	0.48
4:B:1025:COA:CBP	4:B:1025:COA:H10	2.22	0.48
1:A:117:ARG:HD3	1:A:193:MET:HE1	1.96	0.47
1:D:12:CYS:O	1:D:15:PHE:HB2	2.14	0.47
1:A:1:SER:N	1:A:197:ASP:OD2	2.47	0.47
1:A:15:PHE:CG	1:A:37:GLY:HA3	2.50	0.47
1:A:155:THR:HB	2:B:268:LEU:HD22	1.96	0.47
2:B:352:ASN:O	2:B:353:ASN:HB2	2.14	0.47
2:B:289:VAL:O	2:B:290:GLY:C	2.57	0.47
1:D:223:GLU:O	1:D:223:GLU:HG3	2.14	0.47
1:A:27:ALA:HB2	6:A:1652:HOH:O	2.14	0.47
2:E:261:CYS:O	2:E:287:LEU:HB3	2.15	0.47
1:A:121:PRO:HG2	1:A:180:ASP:OD2	2.16	0.46
2:E:230:ARG:CD	6:E:1562:HOH:O	2.62	0.46
2:B:109:TYR:CE2	2:B:133:ILE:HB	2.51	0.46
2:E:346:VAL:CG2	2:E:381:VAL:HG13	2.46	0.46
2:B:272:THR:O	2:B:275:ILE:HG22	2.16	0.46
1:D:46:THR:HA	1:D:50:LEU:O	2.16	0.46
1:D:71:TYR:CE1	1:D:95:ILE:HG13	2.50	0.46
2:E:245:ALA:HB1	2:E:250:LEU:HB2	1.97	0.46
1:A:71:TYR:CE1	1:A:95:ILE:HG13	2.51	0.46
1:A:155:THR:OG1	2:B:268:LEU:HB2	2.15	0.46
2:B:249:GLU:OE2	2:E:28:PRO:HD2	2.15	0.46
1:A:195:GLU:O	1:A:227:LYS:HE3	2.15	0.46
2:B:263:VAL:HG22	2:B:317:ASN:HB3	1.98	0.45
1:A:72:VAL:CG1	1:A:76:PHE:HB2	2.47	0.45
1:A:253:GLY:HA2	2:B:134:GLU:OE2	2.16	0.45
1:A:155:THR:CB	2:B:268:LEU:HB2	2.46	0.45
1:D:223:GLU:HG2	1:D:224:HIS:NE2	2.31	0.45
1:D:121:PRO:HG2	1:D:180:ASP:OD2	2.16	0.45
2:B:24:ALA:O	4:B:1025:COA:H21	2.17	0.45
2:B:30:GLU:HB3	4:B:1025:COA:S1P	2.56	0.45
1:D:159:GLU:CD	2:E:319:PHE:CD2	2.95	0.45
2:E:279:HIS:O	2:E:382:VAL:HG11	2.16	0.45
1:A:248:GLY:O	2:B:116:ARG:NH2	2.46	0.45
1:D:151:SER:HB3	1:D:157:THR:OG1	2.16	0.45
2:E:84:TYR:OH	2:E:132:GLU:HG3	2.17	0.45
2:E:67:GLU:CD	2:E:67:GLU:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:95:GLN:HE21	2:E:95:GLN:HB2	1.48	0.45
2:E:346:VAL:CB	2:E:381:VAL:HG13	2.45	0.44
2:B:279:HIS:O	2:B:382:VAL:HG11	2.17	0.44
1:D:71:TYR:C	4:D:1301:COA:H142	2.43	0.44
2:B:308:ASP:OD1	2:B:310:LYS:HG2	2.17	0.44
2:E:320:GLY:CA	4:E:1325:COA:H32	2.48	0.44
2:B:196:ILE:HG12	2:B:216:LEU:HD22	2.00	0.44
1:D:199:GLN:O	1:D:199:GLN:HG2	2.18	0.44
2:E:352:ASN:HD22	4:E:1325:COA:H71	1.82	0.44
1:A:151:SER:HB3	1:A:157:THR:OG1	2.17	0.44
1:D:15:PHE:CG	1:D:37:GLY:HA3	2.53	0.44
2:E:262:MET:HE1	2:E:302:PHE:CD2	2.52	0.44
1:A:223:GLU:HG2	1:A:224:HIS:NE2	2.32	0.44
2:B:319:PHE:CD1	2:B:319:PHE:C	2.96	0.44
1:A:34:MET:HE3	1:A:34:MET:HB3	1.75	0.43
1:A:71:TYR:C	4:A:1300:COA:H142	2.43	0.43
1:D:11:ILE:HG23	1:D:65:ALA:CB	2.48	0.43
2:E:112:ALA:HA	2:E:122:VAL:O	2.17	0.43
1:A:97:GLU:HB3	4:A:1300:COA:H71	2.00	0.43
2:B:333:ILE:HG23	2:B:366:LEU:CD1	2.48	0.43
2:B:336:VAL:HA	2:B:341:VAL:HG23	2.00	0.43
1:D:222:LYS:HB2	1:D:268:ALA:HB1	2.00	0.43
2:E:263:VAL:HG22	2:E:317:ASN:HB3	2.00	0.43
2:E:290:GLY:O	2:E:291:GLY:C	2.62	0.43
1:A:151:SER:HA	1:A:206:ILE:O	2.18	0.43
2:B:133:ILE:HD12	2:B:133:ILE:HA	1.82	0.43
2:B:261:CYS:O	2:B:287:LEU:HB3	2.19	0.43
2:B:229:LEU:HD23	2:B:232:MET:HE1	2.01	0.43
2:E:29:ARG:O	2:E:32:GLU:HG2	2.17	0.43
2:B:296:GLU:CD	2:B:296:GLU:H	2.27	0.43
2:B:328:ILE:O	2:B:332:ILE:HG13	2.19	0.42
1:D:72:VAL:CG1	1:D:76:PHE:HB2	2.49	0.42
1:A:105:LEU:HD23	1:A:105:LEU:C	2.43	0.42
1:A:157:THR:O	1:A:161:VAL:HG23	2.20	0.42
1:A:181:PRO:CA	2:B:116:ARG:HD3	2.50	0.42
2:E:84:TYR:CE1	2:E:85:GLN:HG3	2.55	0.42
2:B:87:ASP:C	2:B:87:ASP:OD1	2.62	0.42
1:D:67:ALA:HA	1:D:91:LEU:O	2.20	0.42
1:D:151:SER:HA	1:D:206:ILE:O	2.19	0.42
2:B:229:LEU:HD23	2:B:232:MET:HE2	2.01	0.42
2:B:249:GLU:CD	2:E:70:ARG:HH22	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:VAL:HG12	2:B:132:GLU:N	2.34	0.42
2:B:369:ILE:HG21	2:B:380:GLN:OE1	2.20	0.42
1:A:243:ARG:HD2	1:A:247:ALA:HA	2.01	0.42
1:A:9:LYS:HG2	1:A:35:VAL:HG11	2.02	0.42
1:D:90:LYS:HA	1:D:90:LYS:HD3	1.91	0.42
2:B:335:ALA:O	2:B:339:VAL:HB	2.19	0.42
2:B:223:LEU:HD23	2:B:223:LEU:HA	1.83	0.41
2:B:20:PRO:HD3	2:B:211:CYS:O	2.19	0.41
2:E:109:TYR:O	2:E:125:ALA:HA	2.20	0.41
1:A:124:PRO:HG3	1:A:154:GLY:HA2	2.03	0.41
2:E:84:TYR:CD1	2:E:84:TYR:C	2.98	0.41
2:B:191:ARG:HA	2:B:191:ARG:HD2	1.90	0.41
1:A:181:PRO:CB	2:B:116:ARG:HD3	2.51	0.41
2:B:163:LEU:O	2:B:167:LEU:HG	2.21	0.41
2:B:345:VAL:O	2:B:368:ILE:HA	2.20	0.41
1:A:30:TYR:OH	1:A:129:PRO:HA	2.21	0.41
1:D:221:ILE:HA	1:D:225:VAL:HG23	2.02	0.41
1:D:230:VAL:HA	1:D:271:LYS:O	2.21	0.41
2:B:346:VAL:CB	2:B:381:VAL:HG13	2.47	0.41
2:B:346:VAL:CG2	2:B:381:VAL:HG13	2.51	0.41
2:E:20:PRO:HD3	2:E:211:CYS:O	2.21	0.41
2:E:25:CYS:HB3	2:E:30:GLU:HB3	2.03	0.41
2:E:224:PHE:CD1	2:E:224:PHE:C	2.99	0.41
2:E:296:GLU:CD	2:E:296:GLU:H	2.29	0.40
1:A:275:SER:HB3	1:A:278:ASP:OD2	2.21	0.40
2:E:199:ASN:HA	2:E:200:PRO:HA	1.83	0.40
2:B:347:VAL:HG12	2:B:349:LEU:HG	2.03	0.40
1:D:195:GLU:CD	1:D:226:THR:H	2.30	0.40
2:E:23:TYR:HB3	4:E:1025:COA:H22	2.03	0.40
2:E:275:ILE:HD13	2:E:374:LEU:HG	2.03	0.40
1:D:124:PRO:HG3	1:D:154:GLY:HA2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	285/288 (99%)	279 (98%)	6 (2%)	0	100	100
1	D	285/288 (99%)	278 (98%)	7 (2%)	0	100	100
2	B	386/388 (100%)	377 (98%)	6 (2%)	3 (1%)	16	16
2	E	383/388 (99%)	373 (97%)	5 (1%)	5 (1%)	9	8
All	All	1339/1352 (99%)	1307 (98%)	24 (2%)	8 (1%)	21	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	293	ALA
2	E	293	ALA
2	B	257	GLY
2	B	290	GLY
2	E	257	GLY
2	E	291	GLY
2	E	292	GLY
2	E	290	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/218 (100%)	212 (98%)	5 (2%)	44	59
1	D	217/218 (100%)	212 (98%)	5 (2%)	44	59
2	B	298/298 (100%)	285 (96%)	13 (4%)	25	34
2	E	296/298 (99%)	283 (96%)	13 (4%)	25	34
All	All	1028/1032 (100%)	992 (96%)	36 (4%)	32	43

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	GLU
1	A	150	VAL
1	A	255	LYS
1	A	273	VAL
1	A	287	LEU
2	B	1	MET
2	B	70	ARG
2	B	89	ASN
2	B	95	GLN
2	B	132	GLU
2	B	138	GLU
2	B	195	LEU
2	B	282	GLU
2	B	287	LEU
2	B	288	ASP
2	B	342	ASN
2	B	348	ARG
2	B	381	VAL
1	D	113	GLU
1	D	150	VAL
1	D	223	GLU
1	D	255	LYS
1	D	273	VAL
2	E	1	MET
2	E	70	ARG
2	E	89	ASN
2	E	95	GLN
2	E	124	MET
2	E	133	ILE
2	E	138	GLU
2	E	195	LEU
2	E	282	GLU
2	E	287	LEU
2	E	348	ARG
2	E	364	SER
2	E	381	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	19	GLN
1	A	140	HIS

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Mol	Chain	Res	Type
1	A	224	HIS
2	B	95	GLN
2	B	244	GLN
2	B	352	ASN
1	D	7	ASN
1	D	19	GLN
1	D	140	HIS
1	D	224	HIS
2	E	95	GLN
2	E	342	ASN
2	E	352	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
5	SO4	E	1401	-	4,4,4	0.48	0	6,6,6	0.18	0
3	PO4	D	1601	-	4,4,4	1.57	0	6,6,6	0.49	0
4	COA	A	1300	-	47,50,50	1.34	4 (8%)	69,75,75	2.09	15 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	COA	E	1325	2	7,8,50	1.86	2 (28%)	7,8,75	2.54	4 (57%)
3	PO4	A	1600	-	4,4,4	1.44	0	6,6,6	0.44	0
4	COA	E	1025	2	14,17,50	2.32	6 (42%)	19,22,75	3.82	13 (68%)
5	SO4	B	1400	-	4,4,4	0.45	0	6,6,6	0.15	0
5	SO4	E	1501	-	4,4,4	0.52	0	6,6,6	0.33	0
4	COA	B	1325	2	14,17,50	2.53	7 (50%)	19,22,75	4.99	13 (68%)
5	SO4	B	1500	-	4,4,4	0.60	0	6,6,6	0.26	0
4	COA	D	1301	-	47,50,50	1.04	5 (10%)	69,75,75	2.06	11 (15%)
4	COA	B	1025	2	14,17,50	3.30	6 (42%)	19,22,75	3.84	13 (68%)

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
4	COA	A	1300	-	-	2/48/64/64	0/3/3/3
4	COA	E	1325	2	-	1/7/7/64	-
4	COA	E	1025	2	-	11/23/23/64	-
4	COA	B	1325	2	-	4/23/23/64	-
4	COA	D	1301	-	-	4/48/64/64	0/3/3/3
4	COA	B	1025	2	-	11/23/23/64	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1025	COA	CCP-CBP	8.60	1.59	1.53
4	E	1025	COA	CCP-CBP	4.92	1.56	1.53
4	B	1325	COA	C3P-N4P	4.76	1.56	1.46
4	B	1325	COA	C6P-C5P	4.59	1.60	1.51
4	A	1300	COA	OAP-CAP	4.45	1.50	1.42
4	A	1300	COA	C3P-N4P	4.36	1.56	1.46
4	B	1025	COA	OAP-CAP	4.35	1.50	1.42
4	B	1025	COA	C3P-N4P	4.29	1.55	1.46
4	E	1325	COA	C6P-C5P	3.91	1.59	1.51
4	B	1025	COA	C6P-C5P	3.66	1.58	1.51
4	E	1025	COA	C6P-C5P	3.39	1.58	1.51
4	E	1025	COA	OAP-CAP	3.33	1.48	1.42
4	A	1300	COA	P1A-O3A	3.05	1.62	1.59
4	B	1025	COA	CEP-CBP	3.04	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1325	COA	C7P-N8P	2.89	1.52	1.46
4	D	1301	COA	OAP-CAP	2.83	1.47	1.42
4	B	1325	COA	C2P-S1P	2.81	1.91	1.80
4	B	1325	COA	CDP-CBP	2.73	1.59	1.53
4	B	1325	COA	OAP-CAP	2.65	1.47	1.42
4	B	1025	COA	CDP-CBP	2.51	1.58	1.53
4	E	1025	COA	C3P-N4P	2.44	1.51	1.46
4	D	1301	COA	P2A-O3A	2.40	1.62	1.59
4	E	1025	COA	CDP-CBP	2.24	1.58	1.53
4	D	1301	COA	C3P-N4P	2.16	1.51	1.46
4	E	1325	COA	C3P-N4P	2.15	1.51	1.46
4	A	1300	COA	CDP-CBP	2.11	1.58	1.53
4	D	1301	COA	C7P-N8P	2.08	1.50	1.46
4	E	1025	COA	CEP-CBP	2.06	1.58	1.53
4	B	1325	COA	CCP-CBP	2.03	1.55	1.53
4	D	1301	COA	P1A-O3A	2.01	1.61	1.59

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1325	COA	CEP-CBP-CCP	-10.75	86.55	108.77
4	B	1025	COA	CEP-CBP-CAP	9.54	125.04	108.77
4	B	1325	COA	C6P-C5P-N4P	9.34	133.36	116.34
4	E	1025	COA	CEP-CBP-CAP	9.25	124.53	108.77
4	E	1025	COA	CDP-CBP-CCP	-8.21	91.80	108.77
4	B	1025	COA	CDP-CBP-CCP	-8.02	92.21	108.77
4	A	1300	COA	O5P-C5P-C6P	-7.57	108.31	122.02
4	D	1301	COA	O5P-C5P-C6P	-7.45	108.51	122.02
4	A	1300	COA	CEP-CBP-CCP	-7.15	96.43	108.22
4	B	1325	COA	CEP-CBP-CAP	6.86	120.46	108.77
4	B	1325	COA	O5P-C5P-C6P	-6.07	111.01	122.02
4	D	1301	COA	C6P-C5P-N4P	6.07	127.40	116.34
4	D	1301	COA	C3P-N4P-C5P	5.89	133.79	122.82
4	A	1300	COA	CEP-CBP-CAP	5.66	118.42	108.77
4	A	1300	COA	C2P-C3P-N4P	5.66	125.15	112.31
4	B	1325	COA	CAP-C9P-N8P	5.25	126.45	116.48
4	D	1301	COA	C2P-C3P-N4P	5.13	123.94	112.31
4	B	1325	COA	C3P-N4P-C5P	5.12	132.36	122.82
4	E	1025	COA	O9P-C9P-N8P	-5.07	112.26	122.98
4	B	1325	COA	C6P-C7P-N8P	5.05	122.75	112.00
4	D	1301	COA	CEP-CBP-CCP	-5.05	99.89	108.22
4	B	1325	COA	O9P-C9P-N8P	-4.99	112.43	122.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1025	COA	O9P-C9P-N8P	-4.91	112.58	122.98
4	B	1325	COA	OAP-CAP-CBP	-4.66	99.38	110.18
4	E	1325	COA	C7P-C6P-C5P	4.48	120.83	112.37
4	A	1300	COA	C6P-C5P-N4P	4.42	124.40	116.34
4	E	1025	COA	CDP-CBP-CAP	4.36	116.19	108.77
4	D	1301	COA	CDP-CBP-CCP	4.30	115.32	108.22
4	B	1025	COA	CDP-CBP-CAP	4.19	115.92	108.77
4	A	1300	COA	CAP-C9P-N8P	4.09	124.25	116.48
4	B	1025	COA	C7P-N8P-C9P	-4.06	115.25	122.55
4	B	1325	COA	CDP-CBP-CCP	-3.93	100.65	108.77
4	B	1025	COA	C7P-C6P-C5P	3.87	118.84	112.39
4	B	1325	COA	O5P-C5P-N4P	-3.78	115.61	123.03
4	A	1300	COA	CDP-CBP-CCP	3.76	114.44	108.22
4	E	1025	COA	C7P-N8P-C9P	-3.74	115.83	122.55
4	D	1301	COA	CEP-CBP-CAP	3.74	115.14	108.77
4	D	1301	COA	CAP-C9P-N8P	3.71	123.52	116.48
4	B	1325	COA	CDP-CBP-CAP	3.62	114.94	108.77
4	E	1025	COA	C7P-C6P-C5P	3.59	118.37	112.39
4	E	1325	COA	O5P-C5P-N4P	-3.47	116.22	123.03
4	B	1025	COA	O9P-C9P-CAP	3.33	130.19	120.89
4	B	1325	COA	C2P-C3P-N4P	3.27	119.73	112.31
4	E	1025	COA	O9P-C9P-CAP	3.17	129.74	120.89
4	D	1301	COA	O3B-P3B-O7A	-3.15	98.10	109.33
4	E	1025	COA	O5P-C5P-C6P	-3.07	116.45	122.02
4	B	1025	COA	OAP-CAP-CBP	-2.77	103.76	110.18
4	B	1025	COA	O5P-C5P-C6P	-2.73	117.07	122.02
4	B	1025	COA	C2P-C3P-N4P	2.73	118.50	112.31
4	A	1300	COA	C3P-N4P-C5P	2.73	127.90	122.82
4	E	1025	COA	OAP-CAP-C9P	-2.60	98.53	109.38
4	E	1025	COA	CEP-CBP-CCP	-2.43	103.75	108.77
4	E	1025	COA	OAP-CAP-CBP	-2.41	104.60	110.18
4	A	1300	COA	OAP-CAP-CBP	-2.29	104.88	110.18
4	A	1300	COA	C2B-C1B-N9A	2.27	118.94	113.30
4	D	1301	COA	C2B-C1B-N9A	2.23	118.86	113.30
4	E	1325	COA	C6P-C5P-N4P	2.18	120.31	116.34
4	A	1300	COA	O5P-C5P-N4P	2.17	127.29	123.03
4	E	1025	COA	C2P-C3P-N4P	2.15	117.19	112.31
4	B	1025	COA	CEP-CBP-CDP	-2.12	104.98	109.20
4	B	1025	COA	CEP-CBP-CCP	-2.09	104.46	108.77
4	B	1025	COA	OAP-CAP-C9P	-2.08	100.69	109.38
4	A	1300	COA	O9P-C9P-CAP	-2.06	115.13	120.89
4	A	1300	COA	O3A-P2A-O4A	-2.06	104.51	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1300	COA	O3B-P3B-O7A	-2.05	102.02	109.33
4	E	1325	COA	C2P-C3P-N4P	-2.04	107.68	112.31
4	A	1300	COA	OAP-CAP-C9P	2.02	117.82	109.38
4	E	1025	COA	CEP-CBP-CDP	-2.01	105.19	109.20
4	D	1301	COA	O9P-C9P-CAP	-2.00	115.30	120.89

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1300	COA	S1P-C2P-C3P-N4P
4	B	1025	COA	OAP-CAP-CBP-CCP
4	B	1025	COA	C9P-CAP-CBP-CCP
4	B	1025	COA	OAP-CAP-CBP-CDP
4	B	1025	COA	C9P-CAP-CBP-CDP
4	B	1025	COA	OAP-CAP-CBP-CEP
4	B	1025	COA	C9P-CAP-CBP-CEP
4	B	1025	COA	O9P-C9P-CAP-OAP
4	B	1025	COA	N8P-C9P-CAP-OAP
4	B	1025	COA	S1P-C2P-C3P-N4P
4	D	1301	COA	S1P-C2P-C3P-N4P
4	E	1025	COA	OAP-CAP-CBP-CCP
4	E	1025	COA	C9P-CAP-CBP-CCP
4	E	1025	COA	OAP-CAP-CBP-CDP
4	E	1025	COA	C9P-CAP-CBP-CDP
4	E	1025	COA	OAP-CAP-CBP-CEP
4	E	1025	COA	C9P-CAP-CBP-CEP
4	E	1025	COA	O9P-C9P-CAP-OAP
4	E	1025	COA	N8P-C9P-CAP-OAP
4	E	1025	COA	S1P-C2P-C3P-N4P
4	E	1325	COA	C5P-C6P-C7P-N8P
4	B	1325	COA	O9P-C9P-CAP-OAP
4	B	1025	COA	O9P-C9P-CAP-CBP
4	B	1325	COA	O9P-C9P-CAP-CBP
4	E	1025	COA	O9P-C9P-CAP-CBP
4	B	1025	COA	N8P-C9P-CAP-CBP
4	E	1025	COA	N8P-C9P-CAP-CBP
4	B	1325	COA	N8P-C9P-CAP-OAP
4	B	1325	COA	N8P-C9P-CAP-CBP
4	D	1301	COA	O4B-C1B-N9A-C8A
4	D	1301	COA	C2B-C1B-N9A-C8A
4	A	1300	COA	N8P-C9P-CAP-OAP

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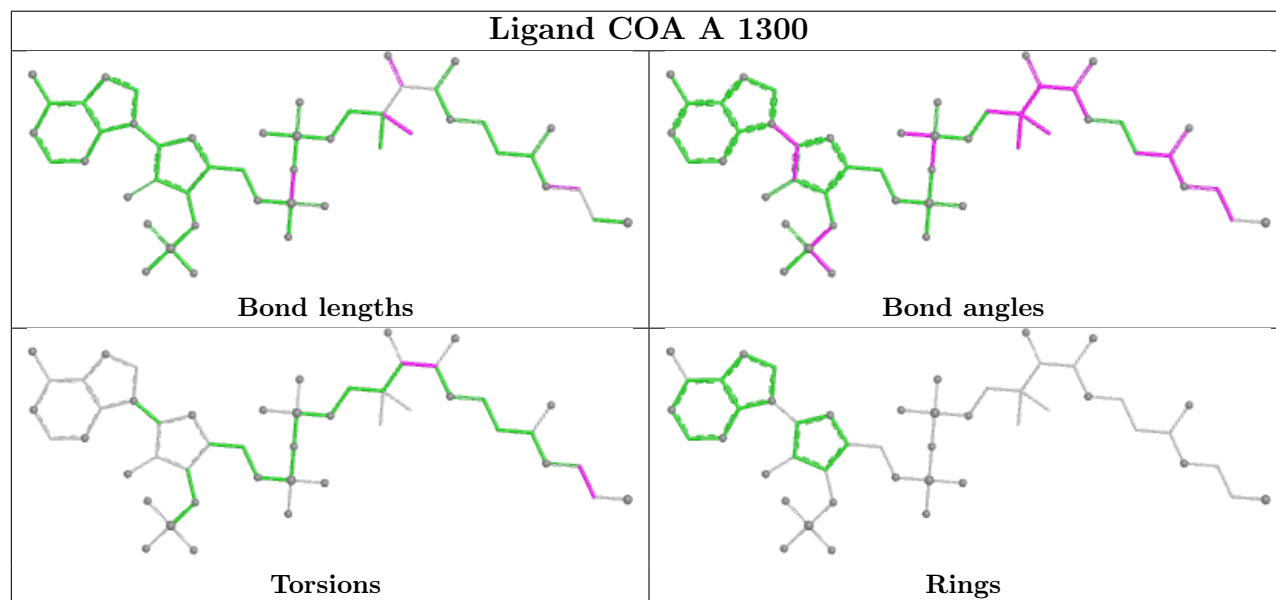
Mol	Chain	Res	Type	Atoms
4	D	1301	COA	N8P-C9P-CAP-OAP

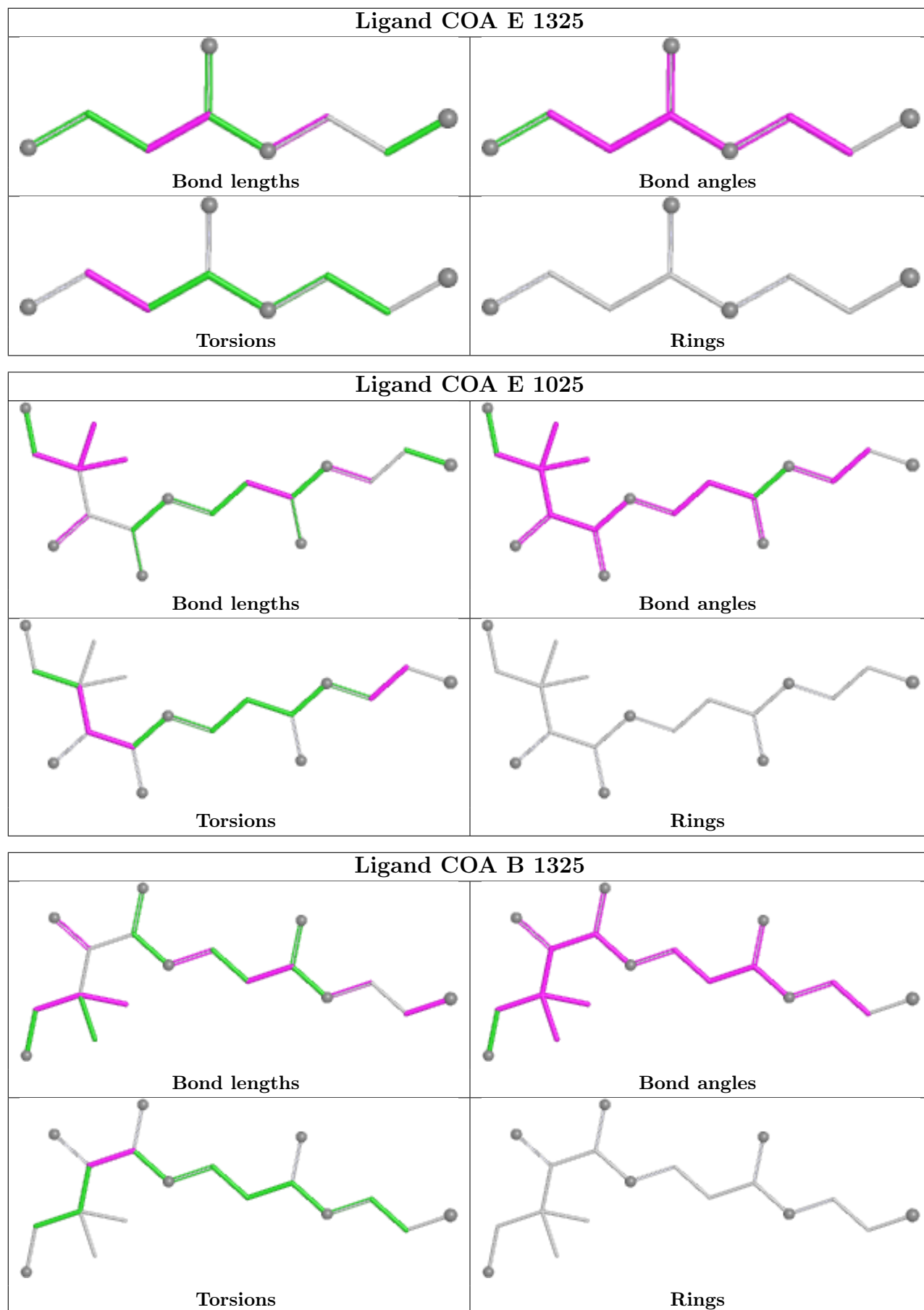
There are no ring outliers.

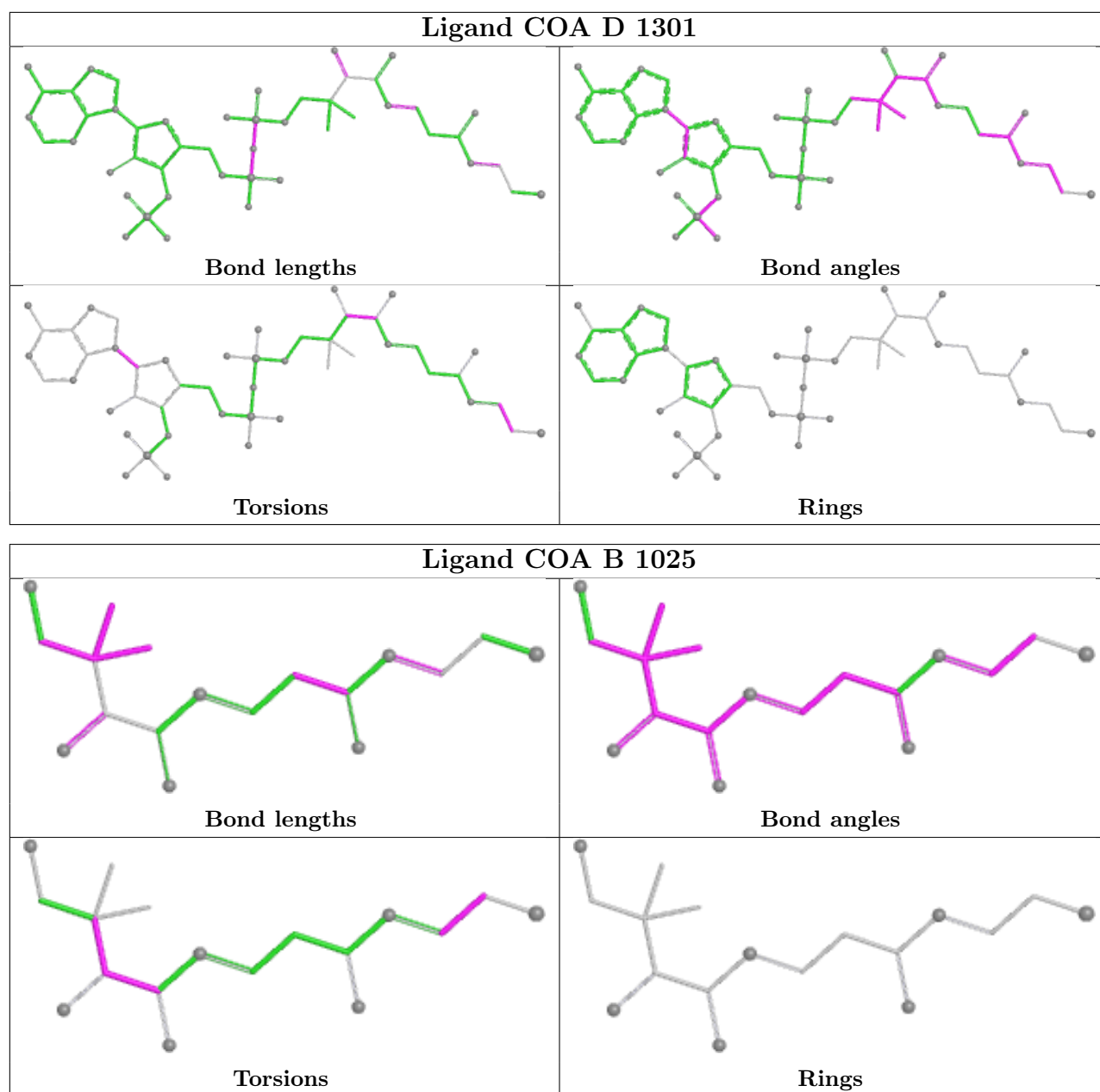
6 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1300	COA	3	0
4	E	1325	COA	3	0
4	E	1025	COA	5	0
4	B	1325	COA	4	0
4	D	1301	COA	2	0
4	B	1025	COA	5	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	287/288 (99%)	-0.26	3 (1%)	79 77	23, 35, 54, 68	0
1	D	287/288 (99%)	0.05	2 (0%)	84 82	24, 41, 59, 69	0
2	B	388/388 (100%)	0.09	14 (3%)	46 43	23, 42, 62, 76	0
2	E	385/388 (99%)	0.22	24 (6%)	26 23	23, 44, 71, 84	0
All	All	1347/1352 (99%)	0.04	43 (3%)	50 47	23, 41, 63, 84	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	293	ALA	5.7
2	E	327	LEU	3.9
2	E	385	VAL	3.8
2	E	330	ASP	3.6
2	B	291	GLY	3.5
2	B	335	ALA	3.3
1	A	287	LEU	3.2
2	E	356	LEU	3.2
1	A	139	GLY	3.0
2	E	291	GLY	3.0
2	B	333	ILE	2.9
2	B	337	ALA	2.9
2	E	383	ALA	2.9
2	B	336	VAL	2.8
2	E	323	VAL	2.8
2	E	384	ALA	2.7
1	A	140	HIS	2.7
2	E	352	ASN	2.6
1	D	186	ASN	2.6
2	E	329	ALA	2.6
2	E	337	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	326	ASP	2.5
2	E	363	ASP	2.4
2	B	313	ALA	2.4
2	B	322	ILE	2.4
2	E	371	ALA	2.3
2	B	339	VAL	2.3
2	B	324	ARG	2.2
1	D	287	LEU	2.2
2	E	324	ARG	2.1
2	B	256	ASP	2.1
2	B	334	GLY	2.1
2	E	67	GLU	2.1
2	E	40	ALA	2.1
2	E	353	ASN	2.1
2	E	289	VAL	2.1
2	E	381	VAL	2.1
2	E	256	ASP	2.0
2	B	289	VAL	2.0
2	E	336	VAL	2.0
2	B	67	GLU	2.0
2	B	374	LEU	2.0
2	E	37	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	COA	E	1025	18/48	0.51	0.28	68,83,84,85	0

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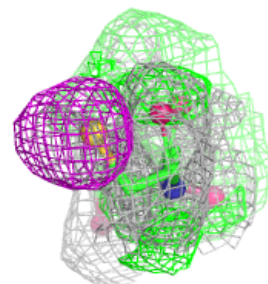
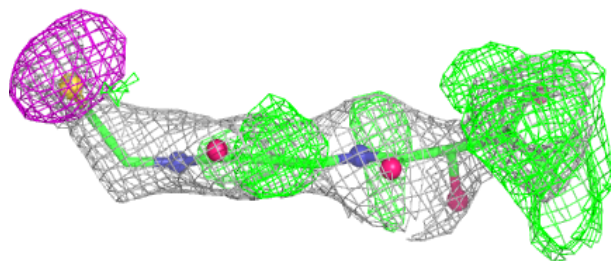
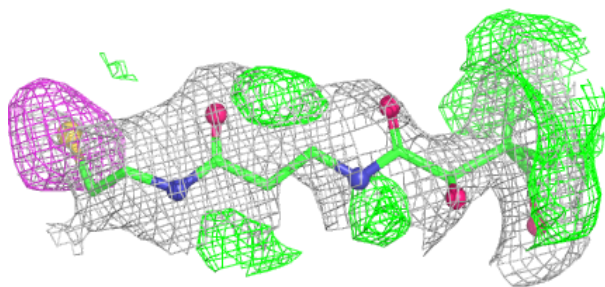
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	COA	B	1025	18/48	0.57	0.26	65,83,87,87	0
4	COA	B	1325	18/48	0.77	0.19	62,74,78,79	0
5	SO4	E	1501	5/5	0.84	0.13	78,80,80,82	0
4	COA	E	1325	9/48	0.85	0.17	65,73,74,74	0
5	SO4	B	1400	5/5	0.86	0.10	79,81,81,82	0
5	SO4	B	1500	5/5	0.90	0.12	69,69,72,72	0
5	SO4	E	1401	5/5	0.92	0.08	66,68,69,70	0
4	COA	D	1301	48/48	0.93	0.09	36,41,53,61	0
4	COA	A	1300	48/48	0.95	0.08	38,41,54,63	0
3	PO4	A	1600	5/5	0.98	0.05	36,39,40,41	0
3	PO4	D	1601	5/5	0.98	0.05	42,43,45,46	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.

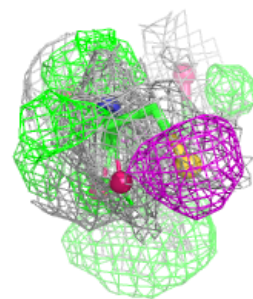
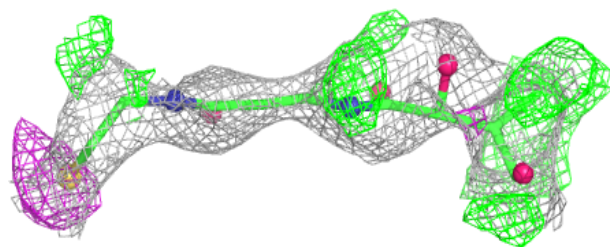
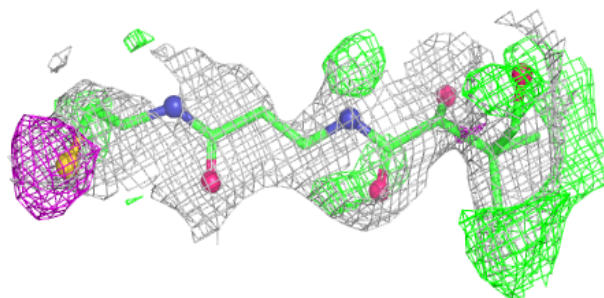
Electron density around COA E 1025:

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

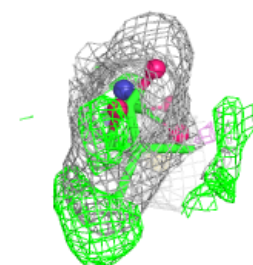
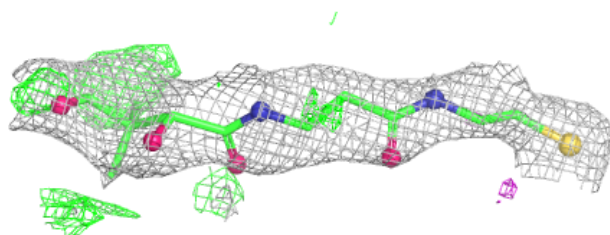
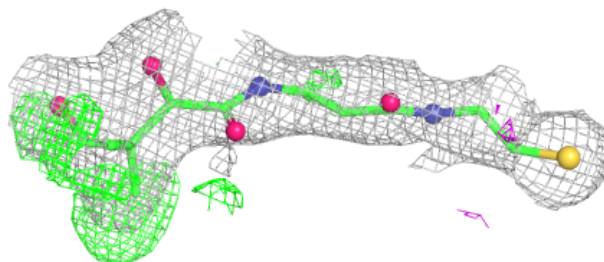


Electron density around COA B 1025:

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

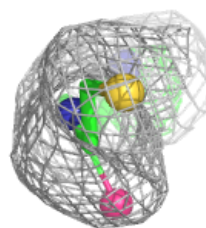
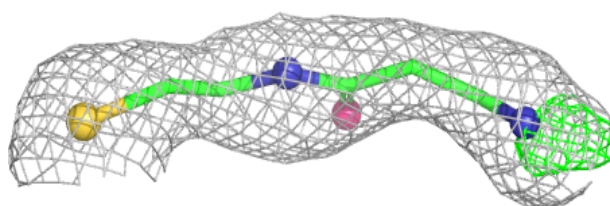
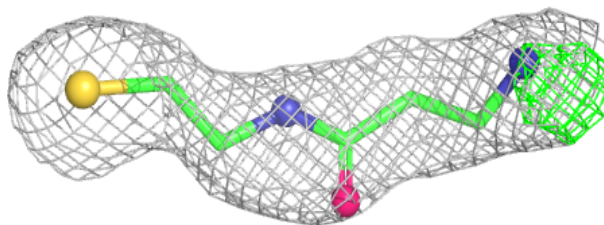
**Electron density around COA B 1325:**

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

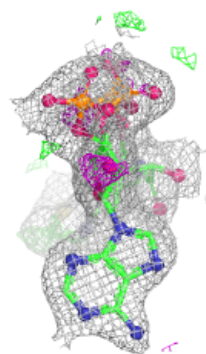
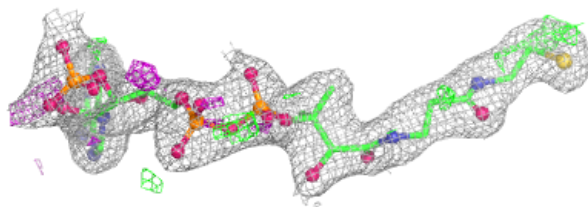
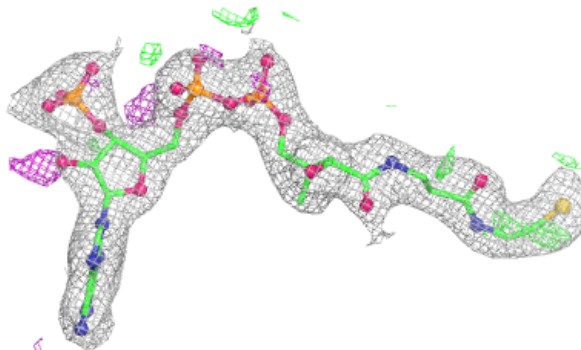


Electron density around COA E 1325:

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

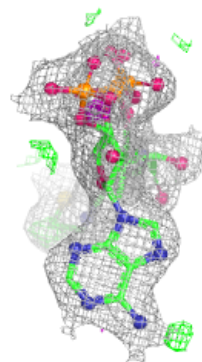
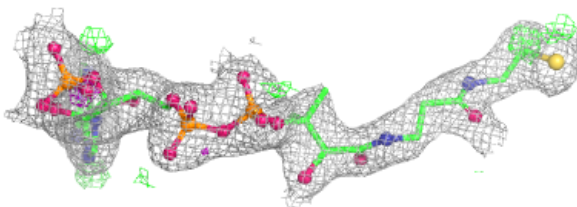
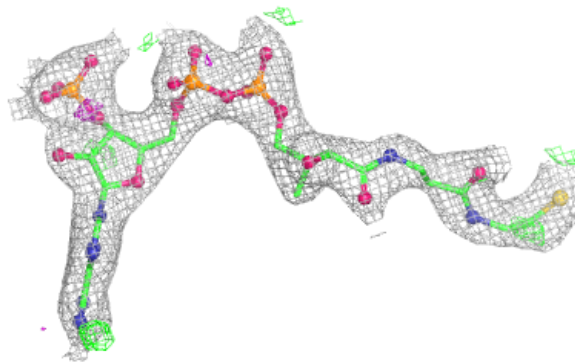
**Electron density around COA D 1301:**

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



Electron density around COA A 1300:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.