



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:09 PM UTC

PDB ID : 4R87 / pdb_00004r87
Title : Crystal structure of spermidine N-acetyltransferase from *Vibrio cholerae* in complex with CoA and spermine
Authors : Filippova, E.V.; Minasov, G.; Kiryukhina, O.; Kuhn, M.L.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2014-08-29
Resolution : 2.61 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

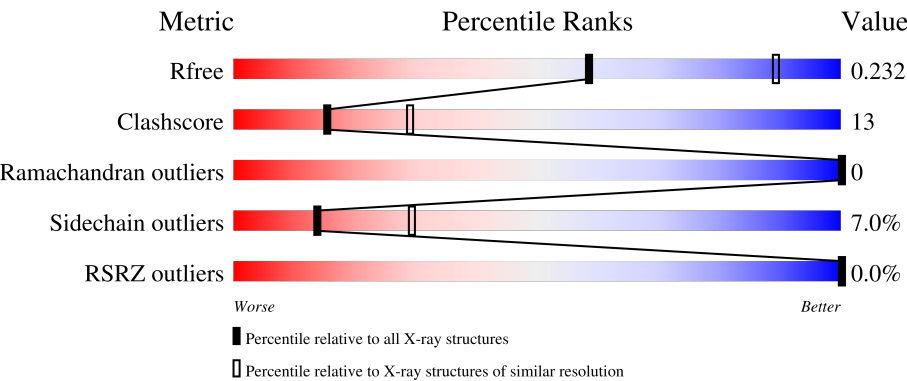
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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 $\leq 5\%$. 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	176	62%32%..
1	B	176	59%35%..
1	C	176	66%27%..
1	D	176	60%32%..5%

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Mol	Chain	Length	Quality of chain
1	E	176	59%34%
1	F	176	% 64%30%
1	G	176	60%35%
1	H	176	69%23%
1	I	176	66%27%
1	J	176	55%39%
1	K	176	58%33%6%
1	L	176	62%30%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18174 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 Spermidine n1-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1439	921	253	262	3			
1	B	169	Total	C	N	O	S	0	1	0
			1437	920	250	264	3			
1	C	169	Total	C	N	O	S	0	0	0
			1423	912	247	261	3			
1	D	168	Total	C	N	O	S	0	0	0
			1420	911	247	259	3			
1	E	170	Total	C	N	O	S	0	0	0
			1439	921	253	262	3			
1	F	169	Total	C	N	O	S	0	0	0
			1428	915	249	261	3			
1	G	170	Total	C	N	O	S	0	1	0
			1447	925	255	264	3			
1	H	169	Total	C	N	O	S	0	0	0
			1428	915	249	261	3			
1	I	169	Total	C	N	O	S	0	0	0
			1428	915	249	261	3			
1	J	169	Total	C	N	O	S	0	1	0
			1439	921	253	262	3			
1	K	170	Total	C	N	O	S	0	0	0
			1439	921	253	262	3			
1	L	169	Total	C	N	O	S	0	0	0
			1428	915	249	261	3			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9KL03
A	-1	ASN	-	expression tag	UNP Q9KL03
A	0	ALA	-	expression tag	UNP Q9KL03
B	-2	SER	-	expression tag	UNP Q9KL03
B	-1	ASN	-	expression tag	UNP Q9KL03

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	expression tag	UNP Q9KL03
C	-2	SER	-	expression tag	UNP Q9KL03
C	-1	ASN	-	expression tag	UNP Q9KL03
C	0	ALA	-	expression tag	UNP Q9KL03
D	-2	SER	-	expression tag	UNP Q9KL03
D	-1	ASN	-	expression tag	UNP Q9KL03
D	0	ALA	-	expression tag	UNP Q9KL03
E	-2	SER	-	expression tag	UNP Q9KL03
E	-1	ASN	-	expression tag	UNP Q9KL03
E	0	ALA	-	expression tag	UNP Q9KL03
F	-2	SER	-	expression tag	UNP Q9KL03
F	-1	ASN	-	expression tag	UNP Q9KL03
F	0	ALA	-	expression tag	UNP Q9KL03
G	-2	SER	-	expression tag	UNP Q9KL03
G	-1	ASN	-	expression tag	UNP Q9KL03
G	0	ALA	-	expression tag	UNP Q9KL03
H	-2	SER	-	expression tag	UNP Q9KL03
H	-1	ASN	-	expression tag	UNP Q9KL03
H	0	ALA	-	expression tag	UNP Q9KL03
I	-2	SER	-	expression tag	UNP Q9KL03
I	-1	ASN	-	expression tag	UNP Q9KL03
I	0	ALA	-	expression tag	UNP Q9KL03
J	-2	SER	-	expression tag	UNP Q9KL03
J	-1	ASN	-	expression tag	UNP Q9KL03
J	0	ALA	-	expression tag	UNP Q9KL03
K	-2	SER	-	expression tag	UNP Q9KL03
K	-1	ASN	-	expression tag	UNP Q9KL03
K	0	ALA	-	expression tag	UNP Q9KL03
L	-2	SER	-	expression tag	UNP Q9KL03
L	-1	ASN	-	expression tag	UNP Q9KL03
L	0	ALA	-	expression tag	UNP Q9KL03

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P		0	0
			41	17	6	15	3			
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	D	1	Total	C	N	O	P		0	0
			41	17	6	15	3			
2	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	G	1	Total	C		O	P		0	0
			21	5		13	3			
2	H	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	I	1	Total	C	N	O	P		0	0
			39	16	5	15	3			
2	J	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	K	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			7	4	3		
4	I	1	Total	C	O	0	0
			7	4	3		
4	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	B	30	Total	O	0	1
			31	31		
5	C	29	Total	O	0	0
			29	29		
5	D	38	Total	O	0	0
			38	38		
5	E	32	Total	O	0	0
			32	32		
5	F	35	Total	O	0	0
			35	35		
5	G	21	Total	O	0	0
			21	21		
5	H	32	Total	O	0	0
			32	32		
5	I	25	Total	O	0	0
			25	25		

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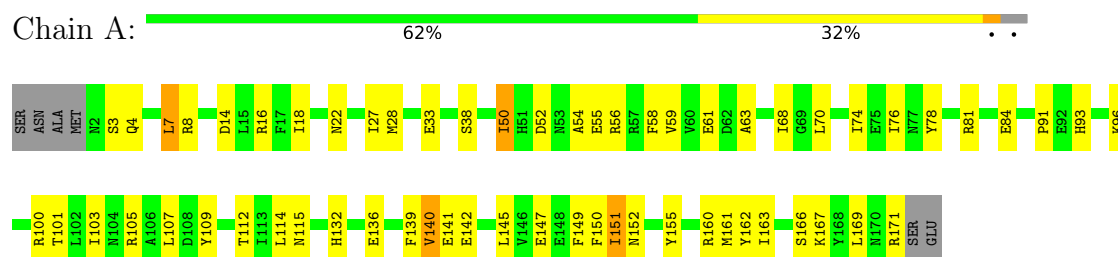
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	31	Total 31	O 31	0	0
5	K	31	Total 31	O 31	0	0
5	L	22	Total 22	O 22	0	0

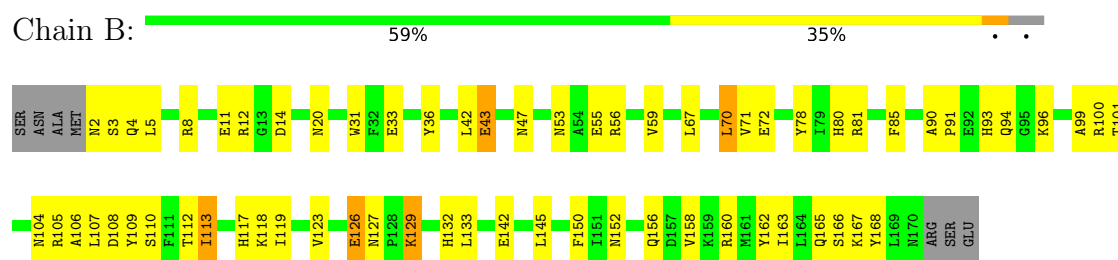
3 Residue-property plots

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.

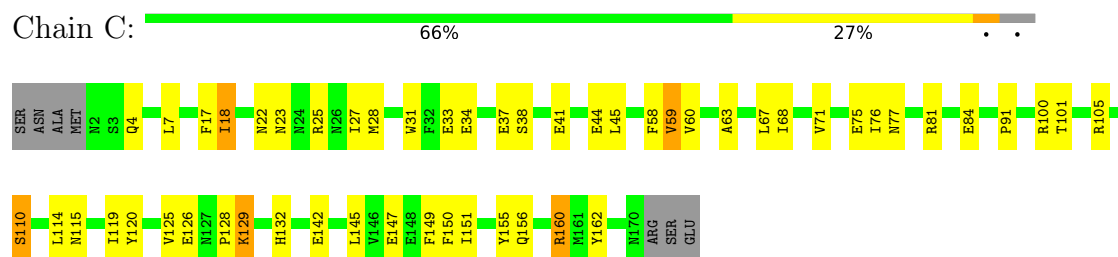
• Molecule 1: Spermidine n1-acetyltransferase



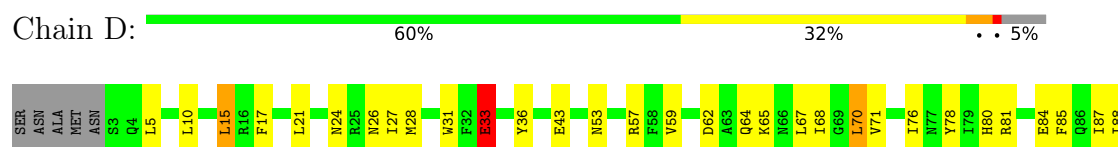
• Molecule 1: Spermidine n1-acetyltransferase

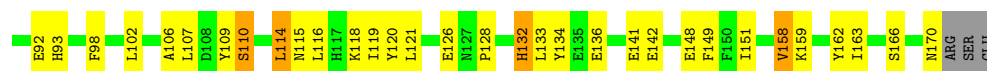


• Molecule 1: Spermidine n1-acetyltransferase



• Molecule 1: Spermidine n1-acetyltransferase

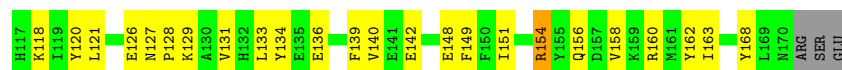




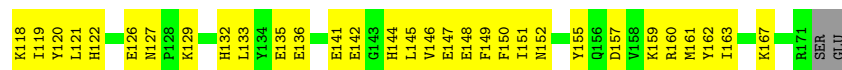
• Molecule 1: Spermidine n1-acetyltransferase



• Molecule 1: Spermidine n1-acetyltransferase



• Molecule 1: Spermidine n1-acetyltransferase

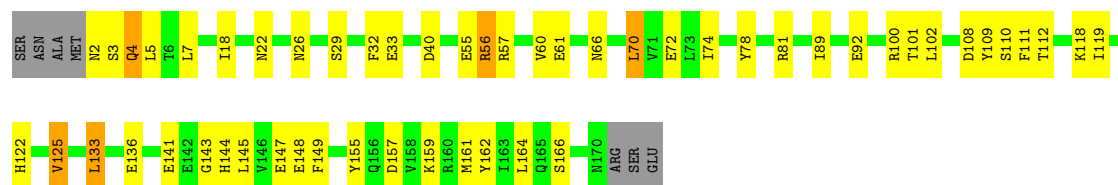


• Molecule 1: Spermidine n1-acetyltransferase

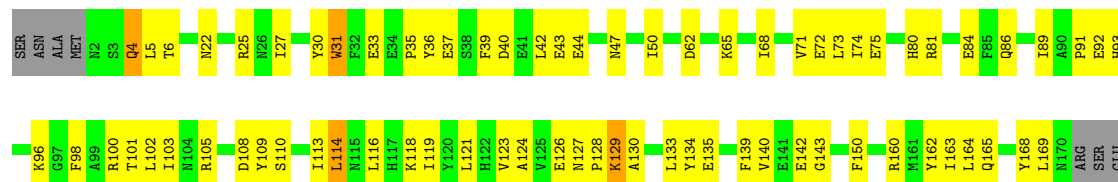


• Molecule 1: Spermidine n1-acetyltransferase

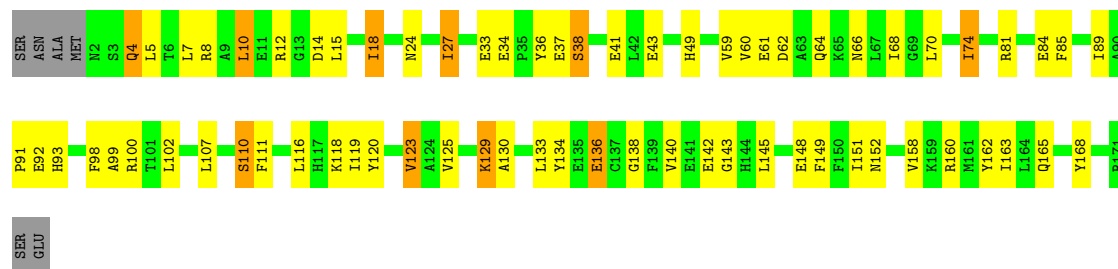




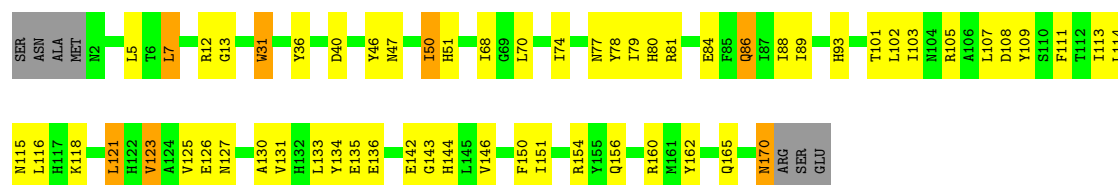
- Molecule 1: Spermidine n1-acetyltransferase



- Molecule 1: Spermidine n1-acetyltransferase



- Molecule 1: Spermidine n1-acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	176.95Å 176.95Å 67.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.82 – 2.61 43.82 – 2.61	Depositor EDS
% Data completeness (in resolution range)	95.7 (43.82-2.61) 89.7 (43.82-2.61)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.185 , 0.238 (Not available) , 0.232	Depositor DCC
R_{free} test set	3390 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 4.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.447 for -h,-k,l 0.440 for h,-h-k,-l 0.437 for -k,-h,-l	Xtriage
Reported twinning fraction	0.271 for H, K, L 0.215 for -K, -H, -L 0.289 for -h,-k,l 0.224 for K, H, -L	Depositor
Outliers	0 of 68098 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18174	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.51% 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: SPM, PEG, COA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.86	0/1472	1.09	3/1987 (0.2%)
1	B	0.93	0/1470	1.11	4/1985 (0.2%)
1	C	0.91	1/1455 (0.1%)	1.07	3/1965 (0.2%)
1	D	0.90	0/1453	1.04	3/1962 (0.2%)
1	E	1.00	0/1472	1.12	1/1987 (0.1%)
1	F	0.97	0/1461	1.08	2/1973 (0.1%)
1	G	1.02	2/1480 (0.1%)	1.14	5/1998 (0.3%)
1	H	0.98	1/1461 (0.1%)	1.18	2/1973 (0.1%)
1	I	0.92	0/1461	1.10	1/1973 (0.1%)
1	J	0.90	0/1472	1.09	3/1987 (0.2%)
1	K	0.93	1/1472 (0.1%)	1.06	2/1987 (0.1%)
1	L	0.89	0/1461	1.13	5/1973 (0.3%)
All	All	0.94	5/17590 (0.0%)	1.10	34/23750 (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	H	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	111	PHE	CA-C	5.35	1.59	1.52
1	C	23	ASN	N-CA	5.17	1.52	1.46
1	G	113	ILE	CA-CB	-5.17	1.50	1.55
1	K	4	GLN	CA-C	5.16	1.57	1.52
1	G	113	ILE	C-O	5.07	1.29	1.23

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	HIS	N-CA-C	8.00	119.69	110.97
1	G	113	ILE	CB-CA-C	-7.75	105.13	111.71
1	L	127	ASN	CA-C-N	7.63	129.38	119.84
1	L	127	ASN	C-N-CA	7.63	129.38	119.84
1	C	76	ILE	N-CA-C	-7.04	94.69	109.34
1	B	43	GLU	N-CA-C	-6.97	103.61	111.07
1	J	103	ILE	N-CA-C	-6.68	104.25	110.53
1	G	113	ILE	N-CA-C	6.38	117.48	111.48
1	E	123	VAL	CB-CA-C	-6.37	100.69	110.50
1	K	18	ILE	CB-CA-C	-6.29	103.78	112.02
1	B	113	ILE	N-CA-C	6.14	116.47	111.62
1	F	68	ILE	N-CA-C	-5.88	107.08	112.96
1	G	17	PHE	N-CA-C	-5.87	104.80	111.14
1	H	49	HIS	N-CA-C	5.84	120.11	112.92
1	K	98	PHE	N-CA-C	5.84	119.58	112.23
1	L	40	ASP	N-CA-C	5.81	117.61	111.28
1	D	43	GLU	N-CA-C	-5.80	104.87	111.14
1	G	71	VAL	N-CA-C	5.74	117.01	108.46
1	A	50	ILE	CB-CA-C	-5.68	104.60	112.04
1	I	56	ARG	N-CA-C	-5.67	101.78	109.95
1	C	129	LYS	N-CA-C	-5.64	105.03	111.07
1	H	169	LEU	N-CA-C	5.55	122.62	110.80
1	C	18	ILE	N-CA-C	-5.54	105.32	110.53
1	B	127	ASN	N-CA-C	-5.53	99.21	108.94
1	J	108	ASP	N-CA-C	-5.48	105.21	111.07
1	J	5	LEU	N-CA-C	5.47	117.65	108.73
1	B	129	LYS	N-CA-C	-5.47	106.66	113.55
1	D	15	LEU	N-CA-C	5.30	119.01	112.54
1	A	68	ILE	CB-CA-C	-5.30	105.26	111.94
1	L	108	ASP	N-CA-C	-5.25	105.46	111.07
1	G	118	LYS	N-CA-C	5.13	115.78	107.32
1	L	123	VAL	CB-CA-C	-5.08	102.91	110.33
1	F	113	ILE	N-CA-C	5.05	116.37	112.12
1	D	33	GLU	CB-CA-C	-5.02	100.44	110.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	169	LEU	Peptide

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	1439	0	1397	36	0
1	B	1437	0	1389	43	0
1	C	1423	0	1379	35	0
1	D	1420	0	1378	48	0
1	E	1439	0	1397	43	0
1	F	1428	0	1384	30	0
1	G	1447	0	1402	46	0
1	H	1428	0	1384	34	0
1	I	1428	0	1384	39	0
1	J	1439	0	1396	57	0
1	K	1439	0	1397	53	0
1	L	1428	0	1384	47	0
2	A	48	0	32	0	0
2	B	41	0	22	3	0
2	C	48	0	32	3	0
2	D	41	0	22	0	0
2	E	48	0	32	2	0
2	F	48	0	32	3	0
2	G	21	0	6	1	0
2	H	48	0	32	1	0
2	I	39	0	21	0	0
2	J	48	0	32	5	0
2	K	48	0	32	1	0
2	L	48	0	32	6	0
3	E	14	0	26	1	0
3	G	14	0	26	0	0
3	H	14	0	26	0	0
3	I	14	0	26	0	0
3	J	14	0	26	1	0
3	K	14	0	26	1	0
4	H	7	0	10	0	0
4	I	7	0	10	0	0
4	L	7	0	10	0	0
5	A	21	0	0	2	0
5	B	31	0	0	1	0
5	C	29	0	0	1	0
5	D	38	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	32	0	0	1	0
5	F	35	0	0	1	0
5	G	21	0	0	1	0
5	H	32	0	0	3	0
5	I	25	0	0	1	0
5	J	31	0	0	0	0
5	K	31	0	0	2	0
5	L	22	0	0	1	0
All	All	18174	0	17184	472	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 13.

All (472) 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:K:129:LYS:HD3	2:K:201:COA:H8A	1.44	0.99
2:C:201:COA:H132	2:C:201:COA:O9P	1.77	0.84
2:L:201:COA:H132	2:L:201:COA:O9P	1.78	0.83
1:I:18:ILE:HD12	1:I:70:LEU:HD11	1.62	0.80
1:F:129:LYS:HG2	2:F:201:COA:O2B	1.83	0.78
1:E:110:SER:HB3	1:E:116:LEU:HD12	1.65	0.77
1:B:109:TYR:CD1	1:B:113:ILE:HD12	2.20	0.76
1:J:30:TYR:CD2	2:J:201:COA:H71	2.22	0.75
1:K:15:LEU:HD23	1:K:18:ILE:HD12	1.68	0.75
1:E:81:ARG:HD3	1:H:81:ARG:HD2	1.68	0.74
1:F:126:GLU:O	1:F:128:PRO:HD3	1.88	0.73
1:K:7:LEU:HD23	1:K:60:VAL:HG22	1.70	0.73
1:I:109:TYR:OH	1:K:36:TYR:HB2	1.90	0.72
1:F:142:GLU:OE2	1:F:160:ARG:NH2	2.21	0.71
1:K:33:GLU:OE2	3:K:202:SPM:N5	2.24	0.71
1:G:146:VAL:O	1:H:118:LYS:NZ	2.20	0.70
1:F:12:ARG:NH1	1:F:47:ASN:OD1	2.24	0.69
1:K:10:LEU:HD11	1:K:18:ILE:HD11	1.74	0.69
1:C:100:ARG:NH1	2:C:201:COA:O7A	2.26	0.68
1:I:56:ARG:NE	1:K:34:GLU:OE1	2.25	0.68
1:J:44:GLU:OE1	1:L:51:HIS:NE2	2.27	0.68
1:J:4:GLN:OE1	1:J:4:GLN:HA	1.93	0.67
1:I:7:LEU:CD2	1:I:60:VAL:HG22	2.24	0.67
2:L:201:COA:O9P	2:L:201:COA:CDP	2.42	0.67
1:I:55:GLU:OE1	1:I:57:ARG:NH1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:GLU:OE1	1:B:156:GLN:HB3	1.96	0.67
1:B:163:ILE:HA	5:B:330:HOH:O	1.95	0.66
1:L:68:ILE:HD13	1:L:93:HIS:CD2	2.29	0.66
1:C:22:ASN:HA	1:C:28:MET:SD	2.35	0.66
1:E:103:ILE:O	1:E:107:LEU:HG	1.96	0.66
1:B:12:ARG:NH1	1:B:47:ASN:OD1	2.29	0.65
1:D:24:ASN:ND2	1:D:27:ILE:HD13	2.12	0.65
1:J:27:ILE:HD11	1:J:91:PRO:HG3	1.78	0.65
1:L:131:VAL:O	1:L:135:GLU:HG3	1.95	0.65
1:L:46:TYR:O	1:L:50:ILE:HG12	1.97	0.64
1:I:7:LEU:HD23	1:I:60:VAL:HG22	1.77	0.64
1:L:5:LEU:O	1:L:105:ARG:NH2	2.31	0.64
1:D:62:ASP:OD1	1:D:65:LYS:N	2.31	0.63
1:B:133:LEU:HD11	2:B:201:COA:H4B	1.79	0.63
1:F:114:LEU:HB3	1:F:116:LEU:HG	1.80	0.63
1:G:84:GLU:HA	1:G:120:TYR:O	1.99	0.63
1:H:51:HIS:ND1	5:H:319:HOH:O	2.30	0.62
1:G:26[B]:ASN:C	1:G:26[B]:ASN:OD1	2.42	0.62
1:J:165:GLN:HG2	1:J:169:LEU:HD12	1.81	0.62
1:K:27:ILE:CD1	1:K:91:PRO:HG3	2.30	0.62
1:E:142:GLU:OE2	1:E:160:ARG:NH2	2.33	0.62
1:I:18:ILE:CD1	1:I:70:LEU:HD11	2.27	0.62
1:I:125:VAL:HG21	1:I:144:HIS:CE1	2.35	0.62
1:G:7:LEU:HD21	1:G:105:ARG:HB3	1.80	0.62
1:I:110:SER:HB3	1:I:119:ILE:HD11	1.80	0.62
1:J:130:ALA:O	1:J:134:TYR:CD2	2.52	0.62
1:K:142:GLU:OE2	1:K:160:ARG:NH2	2.32	0.62
1:D:84:GLU:HA	1:D:120:TYR:O	2.00	0.62
1:I:149:PHE:HD1	1:J:80:HIS:CD2	2.17	0.62
1:E:8:ARG:HE	1:E:61:GLU:CD	2.08	0.61
1:L:116:LEU:O	1:L:165:GLN:HB2	1.99	0.61
1:I:2:ASN:HB3	1:I:4:GLN:HG2	1.82	0.61
1:J:96:LYS:HD2	1:J:98:PHE:CE2	2.35	0.61
1:J:162:TYR:HE2	1:J:164:LEU:HG	1.65	0.61
1:K:62:ASP:OD1	1:K:66:ASN:HB2	2.00	0.61
1:D:142:GLU:OE2	1:D:162:TYR:HB3	2.00	0.61
1:E:89:ILE:HD11	1:E:102:LEU:HD12	1.82	0.61
1:H:110:SER:HB3	1:H:119:ILE:HD11	1.82	0.61
1:D:118:LYS:HE3	1:D:162:TYR:HB2	1.83	0.60
1:E:2:ASN:HB2	5:E:301:HOH:O	2.00	0.60
1:G:145:LEU:N	1:G:145:LEU:CD1	2.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:40:ASP:HB2	1:L:50:ILE:HD12	1.82	0.60
1:D:132:HIS:NE2	1:D:136:GLU:OE2	2.34	0.60
1:H:8:ARG:NE	1:H:61:GLU:OE2	2.35	0.60
1:G:149:PHE:HD1	1:H:80:HIS:CD2	2.19	0.60
2:L:201:COA:O5P	2:L:201:COA:H22	2.01	0.59
1:C:75:GLU:O	1:C:77:ASN:N	2.36	0.59
1:G:145:LEU:N	1:G:145:LEU:HD12	2.17	0.59
1:J:134:TYR:OH	2:J:201:COA:H21	2.02	0.59
1:H:129:LYS:HG3	2:H:201:COA:O4B	2.02	0.59
1:C:110:SER:HB3	1:C:119:ILE:HD11	1.85	0.59
1:E:81:ARG:HD2	1:E:115:ASN:O	2.01	0.59
1:F:121:LEU:HD12	1:F:121:LEU:C	2.28	0.59
1:I:162:TYR:HE1	1:I:164:LEU:HG	1.67	0.59
1:L:109:TYR:CE2	1:L:114:LEU:HD11	2.38	0.59
1:L:133:LEU:HD21	2:L:201:COA:H52A	1.85	0.59
1:G:101:THR:O	1:G:102:LEU:C	2.45	0.58
1:D:76:ILE:HD13	1:D:114:LEU:HD21	1.84	0.58
1:D:141:GLU:OE2	1:D:159:LYS:NZ	2.33	0.58
1:D:166:SER:O	1:D:170:ASN:HB2	2.03	0.58
1:H:32:PHE:HB3	1:H:149:PHE:CD1	2.38	0.58
1:K:4:GLN:O	1:K:4:GLN:HG2	2.04	0.58
1:L:170:ASN:OD1	1:L:170:ASN:N	2.37	0.58
1:D:68:ILE:HA	1:D:93:HIS:HD2	1.68	0.57
1:A:78:TYR:HB3	1:D:78:TYR:CD1	2.38	0.57
1:A:149:PHE:HD1	1:B:80:HIS:CD2	2.22	0.57
1:E:7:LEU:HD23	1:E:60:VAL:HG22	1.86	0.57
1:G:148:GLU:OE1	1:H:160:ARG:NH1	2.36	0.57
1:J:121:LEU:HD23	1:J:139:PHE:CE2	2.39	0.57
1:K:15:LEU:HD23	1:K:18:ILE:CD1	2.33	0.57
1:G:50:ILE:HG22	1:G:51:HIS:HD2	1.70	0.57
1:B:104:ASN:OD1	1:B:168:TYR:HE1	1.88	0.57
1:B:5:LEU:HD12	1:B:101:THR:HG21	1.87	0.57
1:G:71:VAL:HG13	1:G:85:PHE:HE1	1.70	0.57
1:I:5:LEU:HD13	1:I:102:LEU:HD21	1.86	0.57
1:F:118:LYS:HE3	1:F:162:TYR:HB2	1.87	0.56
1:J:4:GLN:OE1	1:J:4:GLN:CA	2.53	0.56
1:L:142:GLU:OE2	1:L:160:ARG:NH2	2.32	0.56
1:I:148:GLU:OE2	1:J:118:LYS:HE2	2.06	0.56
1:D:26:ASN:C	1:D:27:ILE:HD12	2.31	0.56
1:K:123:VAL:HG11	1:K:134:TYR:CE2	2.41	0.56
1:K:123:VAL:HG11	1:K:134:TYR:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LEU:CD1	2:B:201:COA:H4B	2.36	0.55
1:E:134:TYR:HB3	1:E:139:PHE:CD2	2.41	0.55
1:B:118:LYS:HE3	1:B:162:TYR:HB2	1.87	0.55
1:I:78:TYR:HB3	1:L:78:TYR:CD1	2.40	0.55
1:L:12:ARG:NH1	1:L:47:ASN:OD1	2.39	0.55
1:A:78:TYR:CD1	1:D:78:TYR:HB3	2.41	0.55
1:L:109:TYR:CD1	1:L:113:ILE:HD12	2.42	0.55
1:D:85:PHE:CZ	1:D:87:ILE:HB	2.41	0.55
1:J:93:HIS:HA	1:J:96:LYS:HE2	1.89	0.55
1:E:5:LEU:HA	1:E:61:GLU:O	2.07	0.55
1:F:31:TRP:CZ2	1:F:86:GLN:HG3	2.41	0.55
1:A:78:TYR:CG	1:D:78:TYR:HB3	2.41	0.55
1:C:60:VAL:O	1:C:68:ILE:HB	2.07	0.55
1:H:105:ARG:HH21	1:H:105:ARG:HG3	1.72	0.55
1:C:110:SER:CB	1:C:119:ILE:HD11	2.37	0.54
1:I:108:ASP:OD1	1:I:112:THR:HG21	2.07	0.54
1:K:130:ALA:HA	1:K:133:LEU:HB2	1.89	0.54
1:F:100:ARG:NH2	1:F:136:GLU:OE1	2.34	0.54
1:H:64:GLN:N	1:H:64:GLN:OE1	2.41	0.54
1:B:81:ARG:HB3	1:B:117:HIS:H	1.73	0.54
1:F:108:ASP:O	1:F:112:THR:OG1	2.20	0.54
1:G:122:HIS:CE1	1:G:160:ARG:HG2	2.43	0.54
1:K:138:GLY:C	1:K:163:ILE:HD12	2.33	0.54
1:L:121:LEU:HD13	1:L:123:VAL:HG22	1.90	0.53
1:E:78:TYR:CD1	1:H:78:TYR:HB3	2.43	0.53
1:J:127:ASN:N	1:J:128:PRO:CD	2.71	0.53
1:G:126:GLU:HG3	5:G:306:HOH:O	2.06	0.53
1:B:109:TYR:CD1	1:B:113:ILE:CD1	2.90	0.53
1:E:50:ILE:HD13	1:G:40:ASP:HB2	1.91	0.53
1:J:89:ILE:HD11	1:J:102:LEU:HD12	1.91	0.53
1:K:142:GLU:OE1	1:L:146:VAL:N	2.41	0.53
1:B:71:VAL:HG13	1:B:85:PHE:HE1	1.73	0.53
1:G:144:HIS:C	1:G:145:LEU:HD12	2.33	0.53
1:H:53:ASN:C	1:H:78:TYR:OH	2.51	0.53
1:B:93:HIS:HA	1:B:96:LYS:HE3	1.90	0.53
1:E:108:ASP:O	1:E:109:TYR:C	2.49	0.53
1:G:147:GLU:HG2	1:G:155:TYR:HB3	1.91	0.53
1:H:121:LEU:CD1	1:H:123:VAL:HG22	2.39	0.53
1:H:53:ASN:O	1:H:78:TYR:OH	2.26	0.52
1:B:110:SER:HB3	1:B:119:ILE:HD11	1.90	0.52
1:D:68:ILE:HA	1:D:93:HIS:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:LEU:HD13	1:D:163:ILE:HD13	1.90	0.52
1:K:27:ILE:HD12	1:K:91:PRO:HG3	1.91	0.52
1:G:141:GLU:OE2	1:G:159:LYS:NZ	2.40	0.52
1:I:81:ARG:HG3	1:L:115:ASN:ND2	2.25	0.52
1:J:22:ASN:ND2	1:J:37:GLU:OE2	2.42	0.52
1:E:85:PHE:CZ	1:E:103:ILE:HG12	2.44	0.52
1:E:46:TYR:CE2	1:E:50:ILE:HD11	2.45	0.52
1:J:89:ILE:HD11	1:J:102:LEU:CD1	2.40	0.52
1:K:5:LEU:HD13	1:K:102:LEU:HD21	1.91	0.52
1:A:22:ASN:HA	1:A:28:MET:SD	2.50	0.52
1:C:150:PHE:C	1:C:151:ILE:HG13	2.34	0.52
1:E:85:PHE:HZ	1:E:103:ILE:HG12	1.75	0.52
1:G:71:VAL:HG13	1:G:85:PHE:CE1	2.45	0.51
1:J:30:TYR:HB3	2:J:201:COA:O5P	2.09	0.51
1:C:84:GLU:HA	1:C:120:TYR:O	2.10	0.51
1:G:144:HIS:NE2	1:G:157:ASP:OD2	2.40	0.51
1:I:118:LYS:HE3	1:I:162:TYR:HB2	1.93	0.51
1:J:73:LEU:HA	1:J:84:GLU:O	2.10	0.51
1:L:7:LEU:HD22	1:L:105:ARG:HB3	1.93	0.51
1:E:108:ASP:OD1	1:E:108:ASP:C	2.54	0.51
1:E:18:ILE:CD1	1:E:70:LEU:HD21	2.41	0.51
1:K:84:GLU:HA	1:K:120:TYR:O	2.11	0.51
1:J:142:GLU:OE2	1:J:160:ARG:NH2	2.44	0.51
1:J:123:VAL:HG23	2:J:201:COA:S1P	2.51	0.50
1:K:123:VAL:CG1	1:K:134:TYR:HE2	2.25	0.50
1:B:36:TYR:OH	1:D:57:ARG:O	2.21	0.50
1:F:139:PHE:CE1	1:F:163:ILE:HG22	2.46	0.50
1:G:50:ILE:HG22	1:G:51:HIS:CD2	2.46	0.50
1:K:14:ASP:N	1:K:14:ASP:OD1	2.41	0.50
1:K:99:ALA:O	1:K:100:ARG:C	2.53	0.50
1:L:77:ASN:OD1	1:L:77:ASN:C	2.54	0.50
1:F:127:ASN:O	1:F:131:VAL:HG23	2.12	0.50
1:K:89:ILE:HD11	1:K:102:LEU:HD12	1.92	0.50
1:A:147:GLU:HB3	1:A:155:TYR:HB3	1.91	0.50
1:B:150:PHE:CD2	1:D:115:ASN:HB2	2.46	0.50
1:K:110:SER:HB3	1:K:116:LEU:HD12	1.94	0.50
1:B:165:GLN:O	1:B:166:SER:C	2.55	0.50
1:I:143:GLY:HA2	1:J:143:GLY:HA2	1.94	0.50
1:K:123:VAL:CG1	1:K:134:TYR:CE2	2.95	0.50
1:L:142:GLU:HB3	1:L:162:TYR:HD2	1.77	0.50
1:F:134:TYR:OH	2:F:201:COA:H21	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:29:SER:O	1:I:32:PHE:N	2.41	0.50
1:I:141:GLU:HB2	1:I:161:MET:HE3	1.94	0.50
1:A:56:ARG:HB3	1:A:58:PHE:CE2	2.47	0.49
1:B:8:ARG:HH12	1:B:14:ASP:CG	2.20	0.49
1:D:17:PHE:HB2	1:D:67:LEU:HD13	1.93	0.49
1:D:121:LEU:HD21	1:D:134:TYR:CD1	2.47	0.49
1:D:163:ILE:HG23	1:D:163:ILE:O	2.12	0.49
1:J:68:ILE:HA	1:J:93:HIS:CD2	2.48	0.49
1:D:5:LEU:HD13	1:D:102:LEU:HD21	1.95	0.49
1:G:95:GLY:HA2	2:G:201:COA:H51A	1.95	0.49
1:J:31:TRP:HH2	1:J:72:GLU:OE2	1.95	0.49
1:E:129:LYS:HE2	2:E:201:COA:H8A	1.93	0.49
1:K:36:TYR:CD1	1:K:36:TYR:C	2.90	0.49
1:A:140:VAL:O	1:A:161:MET:HA	2.12	0.49
1:B:53:ASN:O	1:B:78:TYR:OH	2.31	0.49
1:E:149:PHE:HD1	1:F:80:HIS:CE1	2.30	0.49
1:G:54:ALA:C	1:G:76:ILE:HD12	2.38	0.49
1:J:36:TYR:HB2	1:L:109:TYR:OH	2.12	0.49
1:F:62:ASP:C	1:F:62:ASP:OD1	2.54	0.49
1:I:145:LEU:HD22	1:J:160:ARG:HD3	1.95	0.49
1:J:74:ILE:HG13	1:J:75:GLU:HG2	1.95	0.49
1:K:100:ARG:NH2	1:K:136:GLU:HB3	2.27	0.49
1:A:78:TYR:HB3	1:D:78:TYR:HB3	1.94	0.49
1:C:145:LEU:HA	1:D:142:GLU:OE1	2.12	0.49
1:F:162:TYR:CD1	1:F:162:TYR:C	2.90	0.48
1:G:7:LEU:HD21	1:G:105:ARG:CB	2.42	0.48
1:E:10:LEU:HD13	1:E:18:ILE:HD11	1.94	0.48
1:K:10:LEU:HD21	1:K:18:ILE:HD11	1.95	0.48
1:B:168:TYR:C	1:B:168:TYR:CD2	2.91	0.48
1:H:121:LEU:CD1	1:H:123:VAL:CG2	2.90	0.48
1:K:74:ILE:HG12	1:K:84:GLU:HB3	1.95	0.48
1:L:89:ILE:HD12	2:L:201:COA:H133	1.93	0.48
1:L:111:PHE:O	1:L:165:GLN:OE1	2.32	0.48
1:C:149:PHE:HB2	1:C:151:ILE:HD11	1.94	0.48
1:K:143:GLY:HA2	1:L:143:GLY:HA2	1.96	0.48
1:L:36:TYR:CD1	1:L:36:TYR:C	2.91	0.48
1:J:68:ILE:HD13	1:J:93:HIS:CD2	2.48	0.48
1:B:71:VAL:HG13	1:B:85:PHE:CE1	2.48	0.48
1:F:62:ASP:OD1	1:F:65:LYS:N	2.46	0.48
1:C:126:GLU:C	1:C:128:PRO:HD3	2.39	0.48
1:A:50:ILE:CD1	1:C:44:GLU:OE1	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:ILE:O	1:F:107:LEU:HG	2.14	0.48
1:G:142:GLU:OE2	1:G:160:ARG:NH2	2.46	0.48
1:K:145:LEU:HB3	1:K:148:GLU:HB2	1.96	0.48
1:A:74:ILE:HG13	1:A:84:GLU:HB3	1.96	0.47
1:B:126:GLU:OE2	1:B:126:GLU:N	2.46	0.47
1:K:10:LEU:HD21	1:K:18:ILE:CD1	2.43	0.47
1:L:150:PHE:C	1:L:151:ILE:HG13	2.38	0.47
1:A:14:ASP:O	1:A:18:ILE:HG12	2.14	0.47
1:A:141:GLU:HA	1:A:160:ARG:O	2.14	0.47
1:D:126:GLU:O	1:D:128:PRO:HD3	2.14	0.47
1:K:149:PHE:HD1	1:L:80:HIS:CD2	2.32	0.47
1:L:101:THR:O	1:L:105:ARG:HG2	2.13	0.47
1:D:114:LEU:HB3	1:D:116:LEU:HG	1.96	0.47
1:J:109:TYR:CD2	1:J:113:ILE:HD12	2.50	0.47
1:C:81:ARG:NH2	1:C:115:ASN:OD1	2.48	0.47
1:D:70:LEU:HD12	1:D:71:VAL:N	2.30	0.47
1:A:167:LYS:HD3	5:A:306:HOH:O	2.14	0.47
1:G:100:ARG:NH1	1:G:136:GLU:OE2	2.42	0.47
1:L:130:ALA:O	1:L:134:TYR:CD2	2.68	0.47
1:A:162:TYR:CD1	1:A:162:TYR:C	2.92	0.47
1:B:105:ARG:HA	1:B:108:ASP:HB3	1.96	0.47
1:L:89:ILE:HD11	1:L:102:LEU:HD12	1.97	0.47
1:B:2:ASN:HB2	1:B:4:GLN:CD	2.40	0.47
1:C:41:GLU:O	1:C:45:LEU:HG	2.15	0.47
1:G:27:ILE:HG23	1:G:88:ILE:HG21	1.97	0.47
1:L:126:GLU:OE1	1:L:154:ARG:NH2	2.41	0.47
1:B:108:ASP:O	1:B:112:THR:OG1	2.30	0.47
1:C:58:PHE:HB2	1:C:71:VAL:HB	1.97	0.47
1:D:106:ALA:O	1:D:110:SER:OG	2.30	0.46
1:F:24:ASN:OD1	1:F:27:ILE:HD13	2.14	0.46
1:G:76:ILE:HG23	1:G:116:LEU:HD21	1.96	0.46
1:I:72:GLU:HB3	1:I:74:ILE:HG23	1.98	0.46
1:F:32:PHE:HD1	1:F:151:ILE:HD11	1.80	0.46
1:D:31:TRP:C	1:D:33:GLU:H	2.22	0.46
1:E:120:TYR:CD1	1:E:160:ARG:NH1	2.84	0.46
1:H:121:LEU:HD13	1:H:123:VAL:HG22	1.97	0.46
1:J:124:ALA:HB3	1:J:127:ASN:HB2	1.95	0.46
1:B:166:SER:OG	1:B:167:LYS:N	2.48	0.46
1:C:101:THR:O	1:C:105:ARG:HG2	2.16	0.46
1:C:147:GLU:HA	1:C:156:GLN:O	2.15	0.46
1:E:15:LEU:HD23	1:E:15:LEU:HA	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:52:ASP:OD2	1:H:55:GLU:OE1	2.34	0.46
1:I:155:TYR:OH	1:J:81:ARG:NH1	2.48	0.46
1:D:110:SER:HB3	1:D:116:LEU:HD12	1.97	0.46
1:G:162:TYR:CD1	1:G:162:TYR:C	2.93	0.46
1:H:64:GLN:N	1:H:64:GLN:CD	2.72	0.46
1:H:149:PHE:CD2	1:H:158:VAL:HG11	2.51	0.46
1:K:27:ILE:HD11	1:K:91:PRO:HG3	1.97	0.46
1:A:76:ILE:HG22	1:A:78:TYR:CZ	2.51	0.46
1:E:128:PRO:O	1:E:131:VAL:N	2.48	0.46
1:J:109:TYR:CE1	1:J:114:LEU:HD13	2.51	0.46
1:J:134:TYR:O	1:J:135:GLU:C	2.59	0.46
1:A:107:LEU:HD21	1:A:139:PHE:HZ	1.80	0.46
1:F:68:ILE:HD13	1:F:93:HIS:CE1	2.50	0.46
1:G:102:LEU:O	1:G:103:ILE:C	2.57	0.46
1:B:81:ARG:NH2	1:B:165:GLN:OE1	2.49	0.46
1:C:149:PHE:HD1	1:D:80:HIS:CD2	2.34	0.46
1:C:160:ARG:NH1	1:D:148:GLU:OE2	2.44	0.46
1:D:110:SER:HB3	1:D:119:ILE:HD11	1.97	0.46
1:H:32:PHE:HD1	1:H:151:ILE:HD11	1.80	0.46
1:I:100:ARG:NH2	1:I:136:GLU:OE1	2.48	0.46
1:J:92:GLU:OE2	1:J:93:HIS:NE2	2.49	0.46
1:B:99:ALA:O	1:B:100:ARG:C	2.58	0.46
1:J:98:PHE:O	1:J:102:LEU:HG	2.16	0.46
1:A:55:GLU:O	1:A:56:ARG:HD3	2.16	0.45
1:A:93:HIS:HA	1:A:96:LYS:HE3	1.97	0.45
1:C:4:GLN:HB2	1:C:63:ALA:HB2	1.99	0.45
1:G:151:ILE:O	1:G:152:ASN:C	2.58	0.45
1:H:10:LEU:HD12	1:H:14:ASP:HB2	1.98	0.45
1:D:71:VAL:HG13	1:D:85:PHE:CE1	2.51	0.45
1:E:27:ILE:HG21	1:E:88:ILE:HG21	1.97	0.45
1:I:149:PHE:HD1	1:J:80:HIS:NE2	2.14	0.45
1:B:123:VAL:O	1:B:123:VAL:HG13	2.17	0.45
1:H:109:TYR:CD2	1:H:113:ILE:HD12	2.52	0.45
1:I:122:HIS:HA	1:I:159:LYS:O	2.16	0.45
1:D:149:PHE:HD2	1:D:158:VAL:HG11	1.80	0.45
1:I:100:ARG:O	1:I:101:THR:C	2.59	0.45
1:J:33:GLU:HG2	3:J:202:SPM:H21	1.99	0.45
1:A:4:GLN:HB2	1:A:63:ALA:HB2	1.98	0.45
1:B:107:LEU:O	1:B:108:ASP:C	2.58	0.45
1:I:29:SER:C	1:I:32:PHE:H	2.25	0.45
1:F:110:SER:HA	1:F:114:LEU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:GLU:OE1	5:H:316:HOH:O	2.20	0.45
1:I:111:PHE:CZ	1:I:119:ILE:HG12	2.51	0.45
1:J:92:GLU:HG3	1:J:93:HIS:CD2	2.51	0.45
1:A:109:TYR:OH	1:C:34:GLU:OE1	2.32	0.45
1:B:94:GLN:HG2	2:B:201:COA:O5A	2.17	0.45
1:G:109:TYR:CD2	1:G:113:ILE:HD12	2.52	0.45
1:A:150:PHE:CD1	1:A:150:PHE:C	2.95	0.45
1:C:17:PHE:HD1	1:C:18:ILE:HD13	1.82	0.45
1:E:7:LEU:CD2	1:E:60:VAL:HG22	2.46	0.45
1:E:31:TRP:CZ2	1:E:86:GLN:HB3	2.51	0.45
1:I:81:ARG:NH1	1:L:81:ARG:HG2	2.30	0.45
1:L:31:TRP:CZ2	1:L:86:GLN:HB2	2.52	0.45
1:L:103:ILE:O	1:L:107:LEU:HG	2.17	0.45
1:B:36:TYR:HB2	1:D:109:TYR:OH	2.16	0.45
1:E:150:PHE:C	1:E:151:ILE:HG13	2.42	0.45
1:H:108:ASP:O	1:H:112:THR:OG1	2.28	0.45
1:L:68:ILE:HA	1:L:93:HIS:CD2	2.52	0.44
1:C:37:GLU:CG	1:C:41:GLU:OE2	2.66	0.44
1:C:142:GLU:HG2	1:C:162:TYR:HD1	1.82	0.44
1:J:150:PHE:CD1	1:L:115:ASN:OD1	2.70	0.44
1:K:37:GLU:HG3	1:K:41:GLU:OE2	2.17	0.44
1:A:112:THR:HG22	1:A:169:LEU:HD21	1.99	0.44
1:E:84:GLU:HA	1:E:120:TYR:O	2.17	0.44
1:G:107:LEU:HD13	1:G:163:ILE:HG21	2.00	0.44
1:A:100:ARG:O	1:A:101:THR:C	2.60	0.44
1:A:27:ILE:HD11	1:A:91:PRO:HD3	1.99	0.44
1:C:27:ILE:HD11	1:C:91:PRO:HD3	1.99	0.44
1:E:41:GLU:OE2	3:E:202:SPM:H121	2.17	0.44
1:E:135:GLU:HG3	1:E:161:MET:HE1	1.99	0.44
1:F:2:ASN:C	1:F:4:GLN:H	2.26	0.44
1:F:111:PHE:CD2	1:F:168:TYR:HB3	2.53	0.44
1:G:150:PHE:C	1:G:151:ILE:HG13	2.43	0.44
1:K:49:HIS:CE1	5:K:314:HOH:O	2.69	0.44
1:K:110:SER:HB3	1:K:119:ILE:HD11	1.98	0.44
1:B:11[B]:GLU:N	1:B:14:ASP:OD2	2.51	0.44
1:J:100:ARG:O	1:J:101:THR:C	2.60	0.44
1:J:127:ASN:N	1:J:128:PRO:HD2	2.32	0.44
1:C:155:TYR:OH	1:D:81:ARG:HD3	2.18	0.44
1:G:135:GLU:HG3	1:G:161:MET:HE1	2.00	0.43
1:K:62:ASP:OD1	1:K:66:ASN:N	2.50	0.43
1:G:144:HIS:O	1:H:142:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:26:ASN:HA	5:I:307:HOH:O	2.17	0.43
1:J:62:ASP:OD1	1:J:65:LYS:N	2.51	0.43
1:A:81:ARG:HD2	1:A:115:ASN:O	2.17	0.43
1:B:42:LEU:O	1:B:43:GLU:C	2.60	0.43
1:B:90:ALA:HB1	1:B:91:PRO:HD2	2.00	0.43
1:E:148:GLU:OE2	1:F:118:LYS:NZ	2.46	0.43
1:A:114:LEU:O	1:A:115:ASN:HB3	2.18	0.43
1:D:114:LEU:O	1:D:115:ASN:HB3	2.17	0.43
1:J:25:ARG:HA	1:J:35:PRO:HB3	2.00	0.43
1:K:15:LEU:CD2	1:K:18:ILE:HD12	2.43	0.43
1:L:12:ARG:O	1:L:13:GLY:C	2.62	0.43
1:K:8:ARG:NH2	1:K:61:GLU:OE1	2.49	0.43
1:C:25:ARG:O	1:C:25:ARG:HG2	2.19	0.43
1:J:109:TYR:O	1:J:110:SER:C	2.60	0.43
1:E:170:ASN:OD1	1:E:170:ASN:N	2.52	0.43
1:F:154:ARG:CZ	1:F:156:GLN:NE2	2.82	0.43
1:G:85:PHE:CZ	1:G:87:ILE:HB	2.53	0.43
1:A:7:LEU:HD21	1:A:105:ARG:CB	2.48	0.43
1:G:122:HIS:ND1	1:G:160:ARG:HG2	2.34	0.43
2:F:201:COA:H72	5:F:311:HOH:O	2.18	0.43
1:B:126:GLU:H	1:B:126:GLU:CD	2.26	0.42
1:C:37:GLU:HG3	1:C:41:GLU:OE2	2.19	0.42
1:D:71:VAL:HG22	1:D:87:ILE:HG13	2.00	0.42
1:E:127:ASN:O	1:E:130:ALA:HB3	2.19	0.42
1:F:84:GLU:HA	1:F:120:TYR:O	2.19	0.42
1:J:43:GLU:O	1:J:47:ASN:ND2	2.52	0.42
1:B:145:LEU:HB2	1:B:158:VAL:HG22	2.01	0.42
1:F:21:LEU:HD13	1:F:88:ILE:HG21	2.01	0.42
1:L:89:ILE:CD1	2:L:201:COA:H133	2.49	0.42
1:A:103:ILE:O	1:A:107:LEU:HG	2.18	0.42
1:A:142:GLU:OE2	1:A:162:TYR:HB3	2.19	0.42
1:A:163:ILE:HA	5:A:306:HOH:O	2.18	0.42
1:D:27:ILE:HD12	1:D:27:ILE:N	2.35	0.42
1:J:6:THR:HA	1:J:105[A]:ARG:NH2	2.34	0.42
1:J:39:PHE:O	1:J:42:LEU:HB3	2.19	0.42
1:B:142:GLU:OE2	1:B:160:ARG:NH2	2.53	0.42
1:C:114:LEU:O	1:C:115:ASN:C	2.61	0.42
1:E:150:PHE:C	1:E:150:PHE:CD1	2.98	0.42
1:E:55:GLU:HA	1:E:73:LEU:O	2.20	0.42
1:I:61:GLU:HG2	1:I:66:ASN:O	2.19	0.42
1:I:147:GLU:N	1:I:157:ASP:OD1	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ILE:HG22	1:A:152:ASN:N	2.34	0.42
1:C:132:HIS:HB3	5:C:317:HOH:O	2.20	0.42
1:D:10:LEU:HD13	1:D:59:VAL:HG23	2.01	0.42
1:L:125:VAL:HG21	1:L:144:HIS:CE1	2.55	0.42
2:C:201:COA:O9P	2:C:201:COA:CDP	2.54	0.42
1:F:148:GLU:HG3	1:F:149:PHE:CE1	2.54	0.42
1:J:129:LYS:HG2	2:J:201:COA:H1B	2.02	0.42
1:K:110:SER:CB	1:K:119:ILE:HD11	2.50	0.42
1:K:168:TYR:CD1	1:K:168:TYR:C	2.98	0.42
1:L:46:TYR:CZ	1:L:50:ILE:HD11	2.55	0.42
1:L:126:GLU:OE1	1:L:156:GLN:OE1	2.38	0.42
1:C:160:ARG:HH12	1:D:148:GLU:CD	2.26	0.42
1:G:110:SER:HB3	1:G:119:ILE:HD11	2.02	0.42
1:B:70:LEU:HD11	1:B:72:GLU:HG3	2.02	0.41
1:D:28:MET:HE3	1:D:33:GLU:HB2	2.01	0.41
1:E:36:TYR:CD1	1:E:36:TYR:C	2.98	0.41
1:K:68:ILE:HA	1:K:93:HIS:CD2	2.56	0.41
1:K:145:LEU:HD22	1:K:158:VAL:HG23	2.02	0.41
1:H:7:LEU:HB3	1:H:58:PHE:CD2	2.55	0.41
1:J:114:LEU:HB3	1:J:116:LEU:HG	2.02	0.41
1:C:17:PHE:CD1	1:C:18:ILE:HD13	2.55	0.41
1:E:71:VAL:HG11	1:E:106:ALA:HB2	2.02	0.41
1:G:27:ILE:HG23	1:G:88:ILE:CG2	2.51	0.41
1:J:168:TYR:CD1	1:J:168:TYR:C	2.98	0.41
1:H:71:VAL:HG22	1:H:87:ILE:HG13	2.02	0.41
1:I:5:LEU:HA	1:I:61:GLU:O	2.19	0.41
1:G:96:LYS:HD2	1:G:98:PHE:CE2	2.56	0.41
1:G:127:ASN:OD1	1:G:129:LYS:HG2	2.21	0.41
1:J:139:PHE:CE2	1:J:163:ILE:HG22	2.55	0.41
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.77	0.41
1:G:121:LEU:C	1:G:121:LEU:HD12	2.46	0.41
1:H:59:VAL:HG11	1:H:67:LEU:HD23	2.02	0.41
1:K:151:ILE:HG22	1:K:152:ASN:OD1	2.21	0.41
1:B:55:GLU:O	1:B:56:ARG:NH2	2.54	0.41
1:B:106:ALA:O	1:B:110:SER:OG	2.27	0.41
1:D:36:TYR:CD1	1:D:36:TYR:C	2.98	0.41
1:E:95:GLY:HA2	2:E:201:COA:H2A	2.03	0.41
1:G:102:LEU:O	1:G:105:ARG:HB2	2.21	0.41
1:H:162:TYR:CD1	1:H:162:TYR:C	2.99	0.41
1:I:100:ARG:HG3	1:I:133:LEU:HD11	2.03	0.41
1:I:145:LEU:CD2	1:J:160:ARG:HD3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:119:ILE:HD13	1:J:119:ILE:HA	1.95	0.41
1:K:37:GLU:HG2	1:K:38:SER:O	2.21	0.41
1:L:162:TYR:CD1	1:L:162:TYR:C	2.99	0.41
1:I:78:TYR:CD1	1:L:78:TYR:HB3	2.57	0.40
1:L:70:LEU:HB3	1:L:88:ILE:HB	2.03	0.40
1:D:15:LEU:HA	1:D:15:LEU:HD23	1.85	0.40
1:D:98:PHE:O	1:D:102:LEU:HG	2.20	0.40
1:E:62:ASP:OD1	1:E:66:ASN:N	2.44	0.40
1:K:81:ARG:NH2	1:K:165:GLN:OE1	2.53	0.40
1:K:111:PHE:CZ	1:K:119:ILE:HG12	2.56	0.40
1:K:118:LYS:HE2	1:K:162:TYR:HB2	2.02	0.40
1:L:118:LYS:HB3	5:L:308:HOH:O	2.22	0.40
1:A:8:ARG:NH2	1:A:61:GLU:OE1	2.54	0.40
1:C:7:LEU:HD22	1:C:60:VAL:HG22	2.02	0.40
1:G:58:PHE:O	1:G:70:LEU:HD12	2.21	0.40
1:J:74:ILE:HG13	1:J:75:GLU:N	2.36	0.40
1:K:10:LEU:CD1	1:K:18:ILE:HD11	2.48	0.40
1:K:12:ARG:HD3	1:K:43:GLU:OE1	2.21	0.40
1:K:24:ASN:ND2	5:K:312:HOH:O	2.55	0.40
1:L:121:LEU:HD13	1:L:123:VAL:CG2	2.51	0.40
1:B:11[A]:GLU:N	1:B:14:ASP:OD2	2.55	0.40
1:C:142:GLU:HG3	1:C:160:ARG:HB3	2.03	0.40
1:D:163:ILE:O	1:D:163:ILE:CG2	2.70	0.40
1:E:124:ALA:HB3	1:E:127:ASN:HB2	2.03	0.40
1:F:8:ARG:O	1:F:58:PHE:HA	2.21	0.40
1:G:89:ILE:O	1:G:90:ALA:C	2.64	0.40
1:G:149:PHE:CD1	1:H:80:HIS:CD2	3.05	0.40
1:J:72:GLU:HB2	1:J:86:GLN:HG3	2.03	0.40
1:A:52:ASP:OD1	1:A:54:ALA:HB3	2.22	0.40
1:A:169:LEU:HD23	1:A:169:LEU:HA	1.95	0.40
1:C:59:VAL:CG1	1:C:67:LEU:HD21	2.51	0.40
1:E:68:ILE:HA	1:E:93:HIS:CD2	2.57	0.40
1:H:28:MET:HE3	1:H:33:GLU:HB3	2.03	0.40
1:H:110:SER:O	1:H:116:LEU:HB2	2.21	0.40
1:H:122:HIS:NE2	5:H:309:HOH:O	2.22	0.40
1:I:111:PHE:CZ	1:I:119:ILE:CG1	3.05	0.40
1:L:74:ILE:HG13	1:L:84:GLU:HB3	2.03	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	168/176 (96%)	150 (89%)	18 (11%)	0	100	100
1	B	168/176 (96%)	148 (88%)	20 (12%)	0	100	100
1	C	167/176 (95%)	152 (91%)	15 (9%)	0	100	100
1	D	166/176 (94%)	150 (90%)	16 (10%)	0	100	100
1	E	168/176 (96%)	155 (92%)	13 (8%)	0	100	100
1	F	167/176 (95%)	156 (93%)	11 (7%)	0	100	100
1	G	169/176 (96%)	153 (90%)	16 (10%)	0	100	100
1	H	167/176 (95%)	150 (90%)	17 (10%)	0	100	100
1	I	167/176 (95%)	153 (92%)	14 (8%)	0	100	100
1	J	168/176 (96%)	145 (86%)	23 (14%)	0	100	100
1	K	168/176 (96%)	146 (87%)	22 (13%)	0	100	100
1	L	167/176 (95%)	148 (89%)	19 (11%)	0	100	100
All	All	2010/2112 (95%)	1806 (90%)	204 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	154/159 (97%)	141 (92%)	13 (8%)	10	21
1	B	154/159 (97%)	143 (93%)	11 (7%)	13	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	152/159 (96%)	144 (95%)	8 (5%)	20	41
1	D	152/159 (96%)	139 (91%)	13 (9%)	10	20
1	E	154/159 (97%)	140 (91%)	14 (9%)	9	18
1	F	153/159 (96%)	142 (93%)	11 (7%)	13	28
1	G	155/159 (98%)	149 (96%)	6 (4%)	28	53
1	H	153/159 (96%)	144 (94%)	9 (6%)	18	36
1	I	153/159 (96%)	142 (93%)	11 (7%)	13	28
1	J	154/159 (97%)	145 (94%)	9 (6%)	18	37
1	K	154/159 (97%)	138 (90%)	16 (10%)	7	13
1	L	153/159 (96%)	145 (95%)	8 (5%)	21	42
All	All	1841/1908 (96%)	1712 (93%)	129 (7%)	14	29

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	7	LEU
1	A	16	ARG
1	A	33	GLU
1	A	38	SER
1	A	59	VAL
1	A	70	LEU
1	A	136	GLU
1	A	140	VAL
1	A	145	LEU
1	A	151	ILE
1	A	166	SER
1	A	171	ARG
1	B	3	SER
1	B	20	ASN
1	B	31	TRP
1	B	33	GLU
1	B	59	VAL
1	B	67	LEU
1	B	70	LEU
1	B	126	GLU
1	B	129	LYS
1	B	132	HIS

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Mol	Chain	Res	Type
1	B	152	ASN
1	C	31	TRP
1	C	33	GLU
1	C	38	SER
1	C	59	VAL
1	C	110	SER
1	C	125	VAL
1	C	129	LYS
1	C	160	ARG
1	D	21	LEU
1	D	33	GLU
1	D	53	ASN
1	D	64	GLN
1	D	70	LEU
1	D	88	ILE
1	D	92	GLU
1	D	110	SER
1	D	114	LEU
1	D	132	HIS
1	D	133	LEU
1	D	151	ILE
1	D	158	VAL
1	E	28	MET
1	E	29	SER
1	E	33	GLU
1	E	50	ILE
1	E	67	LEU
1	E	103	ILE
1	E	108	ASP
1	E	110	SER
1	E	123	VAL
1	E	125	VAL
1	E	129	LYS
1	E	166	SER
1	E	170	ASN
1	E	171	ARG
1	F	3	SER
1	F	16	ARG
1	F	27	ILE
1	F	79	ILE
1	F	94	GLN
1	F	110	SER

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Mol	Chain	Res	Type
1	F	114	LEU
1	F	133	LEU
1	F	140	VAL
1	F	154	ARG
1	F	158	VAL
1	G	7	LEU
1	G	33	GLU
1	G	64	GLN
1	G	132	HIS
1	G	133	LEU
1	G	167	LYS
1	H	5	LEU
1	H	26	ASN
1	H	33	GLU
1	H	79	ILE
1	H	87	ILE
1	H	123	VAL
1	H	129	LYS
1	H	158	VAL
1	H	166	SER
1	I	3	SER
1	I	4	GLN
1	I	22	ASN
1	I	33	GLU
1	I	40	ASP
1	I	70	LEU
1	I	89	ILE
1	I	92	GLU
1	I	125	VAL
1	I	133	LEU
1	I	166	SER
1	J	4	GLN
1	J	31	TRP
1	J	50	ILE
1	J	71	VAL
1	J	114	LEU
1	J	126	GLU
1	J	129	LYS
1	J	133	LEU
1	J	140	VAL
1	K	10	LEU
1	K	27	ILE

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Mol	Chain	Res	Type
1	K	38	SER
1	K	59	VAL
1	K	64	GLN
1	K	70	LEU
1	K	74	ILE
1	K	85	PHE
1	K	92	GLU
1	K	107	LEU
1	K	110	SER
1	K	123	VAL
1	K	125	VAL
1	K	129	LYS
1	K	136	GLU
1	K	140	VAL
1	L	7	LEU
1	L	31	TRP
1	L	50	ILE
1	L	79	ILE
1	L	86	GLN
1	L	121	LEU
1	L	136	GLU
1	L	170	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	104	ASN
1	B	20	ASN
1	B	23	ASN
1	B	51	HIS
1	B	94	GLN
1	B	132	HIS
1	C	22	ASN
1	C	26	ASN
1	C	51	HIS
1	C	53	ASN
1	C	132	HIS
1	D	49	HIS
1	D	66	ASN
1	D	93	HIS
1	D	117	HIS

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Mol	Chain	Res	Type
1	E	93	HIS
1	F	94	GLN
1	F	156	GLN
1	G	22	ASN
1	G	115	ASN
1	G	165	GLN
1	H	4	GLN
1	H	49	HIS
1	I	4	GLN
1	I	22	ASN
1	I	23	ASN
1	I	26	ASN
1	I	115	ASN
1	J	94	GLN
1	K	2	ASN
1	K	49	HIS
1	K	80	HIS
1	K	93	HIS
1	K	117	HIS
1	L	53	ASN
1	L	80	HIS
1	L	93	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	COA	K	201	-	47,50,50	1.39	7 (14%)	69,75,75	2.64	19 (27%)
2	COA	L	201	-	47,50,50	1.48	8 (17%)	69,75,75	2.55	16 (23%)
2	COA	B	201	-	41,43,50	1.39	6 (14%)	62,67,75	2.80	18 (29%)
4	PEG	L	202	-	6,6,6	0.64	0	5,5,5	0.41	0
4	PEG	I	203	-	6,6,6	0.46	0	5,5,5	0.18	0
3	SPM	K	202	-	13,13,13	0.41	0	12,12,12	0.86	0
3	SPM	G	202	-	13,13,13	0.46	0	12,12,12	0.91	0
2	COA	G	201	-	20,21,50	1.03	2 (10%)	30,33,75	1.36	2 (6%)
2	COA	H	201	-	47,50,50	1.53	8 (17%)	69,75,75	2.50	21 (30%)
3	SPM	E	202	-	13,13,13	0.45	0	12,12,12	0.85	0
2	COA	D	201	-	41,43,50	1.56	6 (14%)	62,67,75	3.25	18 (29%)
2	COA	C	201	-	47,50,50	1.33	6 (12%)	69,75,75	2.59	16 (23%)
3	SPM	H	202	-	13,13,13	0.42	0	12,12,12	1.05	1 (8%)
2	COA	E	201	-	47,50,50	1.24	4 (8%)	69,75,75	2.91	25 (36%)
2	COA	F	201	-	47,50,50	1.38	7 (14%)	69,75,75	2.55	18 (26%)
2	COA	J	201	-	47,50,50	1.38	6 (12%)	69,75,75	2.89	22 (31%)
2	COA	I	201	-	40,41,50	1.53	4 (10%)	59,64,75	2.86	18 (30%)
3	SPM	J	202	-	13,13,13	0.45	0	12,12,12	1.22	1 (8%)
4	PEG	H	203	-	6,6,6	0.46	0	5,5,5	0.30	0
3	SPM	I	202	-	13,13,13	0.50	0	12,12,12	1.00	0
2	COA	A	201	-	47,50,50	1.54	10 (21%)	69,75,75	2.73	18 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	K	201	-	-	10/48/64/64	0/3/3/3
2	COA	L	201	-	-	21/48/64/64	0/3/3/3
2	COA	B	201	-	-	11/40/56/64	0/3/3/3
4	PEG	L	202	-	-	1/4/4/4	-
4	PEG	I	203	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SPM	K	202	-	-	4/11/11/11	-
3	SPM	G	202	-	-	6/11/11/11	-
2	COA	G	201	-	-	6/17/30/64	0/1/1/3
2	COA	H	201	-	-	13/48/64/64	0/3/3/3
3	SPM	E	202	-	-	9/11/11/11	-
2	COA	D	201	-	-	14/40/56/64	0/3/3/3
2	COA	C	201	-	-	22/48/64/64	0/3/3/3
3	SPM	H	202	-	-	7/11/11/11	-
2	COA	E	201	-	-	13/48/64/64	0/3/3/3
2	COA	F	201	-	-	17/48/64/64	0/3/3/3
2	COA	J	201	-	-	15/48/64/64	0/3/3/3
2	COA	I	201	-	-	9/33/52/64	0/3/3/3
3	SPM	J	202	-	-	7/11/11/11	-
4	PEG	H	203	-	-	2/4/4/4	-
3	SPM	I	202	-	-	8/11/11/11	-
2	COA	A	201	-	-	5/48/64/64	0/3/3/3

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	201	COA	C5A-C4A	5.32	1.48	1.39
2	A	201	COA	C5A-C4A	5.27	1.48	1.39
2	K	201	COA	C5A-C4A	5.24	1.48	1.39
2	F	201	COA	C5A-C4A	5.21	1.48	1.39
2	L	201	COA	C5A-C4A	5.17	1.48	1.39
2	J	201	COA	C5A-C4A	5.16	1.48	1.39
2	D	201	COA	C5A-C4A	4.99	1.48	1.39
2	B	201	COA	C5A-C4A	4.90	1.47	1.39
2	H	201	COA	C5A-C4A	4.89	1.47	1.39
2	E	201	COA	C5A-C4A	4.77	1.47	1.39
2	C	201	COA	C5A-C4A	4.66	1.47	1.39
2	H	201	COA	P2A-O3A	4.02	1.63	1.59
2	A	201	COA	P1A-O3A	3.68	1.63	1.59
2	H	201	COA	P1A-O3A	3.68	1.63	1.59
2	D	201	COA	P1A-O3A	3.58	1.63	1.59
2	I	201	COA	C5A-C6A	3.52	1.50	1.41
2	I	201	COA	CBP-CAP	3.35	1.59	1.55
2	D	201	COA	P2A-O3A	3.34	1.63	1.59
2	L	201	COA	P1A-O3A	3.34	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	COA	C5A-C6A	3.33	1.50	1.41
2	D	201	COA	C5A-C6A	3.27	1.50	1.41
2	L	201	COA	C5A-C6A	3.25	1.50	1.41
2	J	201	COA	P1A-O3A	3.14	1.62	1.59
2	F	201	COA	C5A-C6A	3.13	1.49	1.41
2	A	201	COA	CCP-CBP	-3.12	1.47	1.52
2	A	201	COA	P2A-O3A	3.10	1.62	1.59
2	A	201	COA	C5A-C6A	3.01	1.49	1.41
2	J	201	COA	C5A-C6A	2.99	1.49	1.41
2	C	201	COA	P1A-O3A	2.94	1.62	1.59
2	L	201	COA	P2A-O3A	2.94	1.62	1.59
2	L	201	COA	CDP-CBP	-2.86	1.47	1.53
2	K	201	COA	C5A-C6A	2.81	1.48	1.41
2	E	201	COA	C5A-C6A	2.77	1.48	1.41
2	F	201	COA	P2A-O3A	2.75	1.62	1.59
2	H	201	COA	C5A-C6A	2.75	1.48	1.41
2	B	201	COA	CEP-CBP	-2.72	1.48	1.53
2	I	201	COA	C8A-N7A	2.67	1.36	1.31
2	B	201	COA	C5A-C6A	2.65	1.48	1.41
2	H	201	COA	C8A-N7A	2.53	1.36	1.31
2	F	201	COA	C8A-N7A	2.52	1.36	1.31
2	K	201	COA	C5A-N7A	-2.50	1.34	1.39
2	K	201	COA	P2A-O3A	2.49	1.62	1.59
2	D	201	COA	C8A-N7A	2.48	1.36	1.31
2	A	201	COA	C8A-N7A	2.48	1.36	1.31
2	G	201	COA	P1A-O3A	2.47	1.62	1.59
2	C	201	COA	C5A-N7A	-2.46	1.34	1.39
2	G	201	COA	P3B-O3B	2.44	1.63	1.59
2	B	201	COA	P1A-O3A	2.44	1.62	1.59
2	L	201	COA	C8A-N7A	2.40	1.36	1.31
2	D	201	COA	P3B-O3B	2.38	1.63	1.59
2	J	201	COA	C8A-N7A	2.36	1.36	1.31
2	C	201	COA	C8A-N7A	2.32	1.36	1.31
2	F	201	COA	CDP-CBP	-2.31	1.49	1.53
2	E	201	COA	C5A-N7A	-2.28	1.34	1.39
2	L	201	COA	C5A-N7A	-2.28	1.34	1.39
2	H	201	COA	C5A-N7A	-2.28	1.34	1.39
2	E	201	COA	C8A-N7A	2.26	1.36	1.31
2	J	201	COA	C5A-N7A	-2.26	1.35	1.39
2	A	201	COA	CDP-CBP	-2.23	1.49	1.53
2	B	201	COA	C8A-N7A	2.21	1.35	1.31
2	H	201	COA	OAP-CAP	2.21	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	201	COA	P1A-O3A	2.20	1.61	1.59
2	H	201	COA	CEP-CBP	-2.19	1.49	1.53
2	K	201	COA	P3B-O3B	2.19	1.63	1.59
2	J	201	COA	P2A-O3A	2.16	1.61	1.59
2	K	201	COA	C8A-N7A	2.13	1.35	1.31
2	F	201	COA	C5A-N7A	-2.13	1.35	1.39
2	A	201	COA	C5A-N7A	-2.12	1.35	1.39
2	L	201	COA	C1B-N9A	2.11	1.52	1.46
2	A	201	COA	C1B-N9A	2.10	1.52	1.46
2	K	201	COA	OAP-CAP	2.09	1.46	1.42
2	A	201	COA	CEP-CBP	-2.06	1.49	1.53
2	B	201	COA	C5A-N7A	-2.03	1.35	1.39
2	C	201	COA	C1B-N9A	2.01	1.51	1.46

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	COA	CEP-CBP-CCP	11.34	126.95	108.22
2	L	201	COA	CDP-CBP-CCP	11.32	126.90	108.22
2	D	201	COA	CAP-C9P-N8P	11.18	123.60	116.32
2	J	201	COA	CDP-CBP-CAP	-11.17	89.72	108.77
2	E	201	COA	CDP-CBP-CAP	-10.50	90.86	108.77
2	D	201	COA	CDP-CBP-CAP	-10.12	91.51	108.77
2	C	201	COA	CDP-CBP-CCP	9.74	124.30	108.22
2	E	201	COA	CEP-CBP-CCP	9.66	124.18	108.22
2	J	201	COA	CDP-CBP-CCP	9.57	124.03	108.22
2	E	201	COA	CEP-CBP-CAP	-9.55	92.49	108.77
2	K	201	COA	CEP-CBP-CAP	-9.36	92.81	108.77
2	H	201	COA	CDP-CBP-CAP	-9.03	93.37	108.77
2	D	201	COA	CDP-CBP-CCP	9.03	123.13	108.22
2	I	201	COA	CDP-CBP-CAP	-8.92	92.77	109.51
2	H	201	COA	CDP-CBP-CCP	8.87	122.87	108.22
2	F	201	COA	CEP-CBP-CDP	8.80	126.75	109.20
2	B	201	COA	CDP-CBP-CCP	8.79	122.73	108.22
2	B	201	COA	CDP-CBP-CAP	-8.59	94.13	108.77
2	I	201	COA	CEP-CBP-CAP	-8.10	94.32	109.51
2	K	201	COA	CDP-CBP-CAP	-8.01	95.11	108.77
2	C	201	COA	CDP-CBP-CAP	-7.99	95.15	108.77
2	D	201	COA	CEP-CBP-CAP	-7.84	95.41	108.77
2	C	201	COA	C5A-C4A-N3A	-7.78	116.01	126.72
2	L	201	COA	C5A-C4A-N3A	-7.65	116.19	126.72
2	F	201	COA	CDP-CBP-CAP	-7.50	95.98	108.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	201	COA	CDP-CBP-CAP	-7.48	96.03	108.77
2	I	201	COA	CEP-CBP-CDP	7.45	124.06	109.20
2	J	201	COA	CEP-CBP-CAP	-7.33	96.27	108.77
2	F	201	COA	CDP-CBP-CCP	7.27	120.22	108.22
2	K	201	COA	CEP-CBP-CDP	7.11	123.38	109.20
2	F	201	COA	O6A-CCP-CBP	7.07	121.91	110.55
2	D	201	COA	C5A-C4A-N3A	-6.94	117.16	126.72
2	D	201	COA	CEP-CBP-CDP	6.90	122.96	109.20
2	E	201	COA	CDP-CBP-CCP	6.76	119.38	108.22
2	B	201	COA	O6A-CCP-CBP	6.69	121.30	110.55
2	A	201	COA	C5A-C4A-N3A	-6.61	117.62	126.72
2	A	201	COA	CEP-CBP-CDP	-6.50	96.25	109.20
2	F	201	COA	C5A-C4A-N3A	-6.48	117.79	126.72
2	B	201	COA	C5A-C4A-N3A	-6.46	117.82	126.72
2	K	201	COA	C5A-C4A-N3A	-6.41	117.89	126.72
2	I	201	COA	C5A-C4A-N3A	-6.22	118.15	126.72
2	K	201	COA	CEP-CBP-CCP	6.21	118.48	108.22
2	I	201	COA	CEP-CBP-CCP	6.12	118.33	108.22
2	J	201	COA	C5A-C4A-N3A	-6.12	118.29	126.72
2	A	201	COA	CEP-CBP-CAP	5.98	118.96	108.77
2	L	201	COA	N3A-C4A-N9A	5.87	137.15	127.17
2	A	201	COA	CDP-CBP-CAP	-5.82	98.84	108.77
2	J	201	COA	CEP-CBP-CDP	5.82	120.80	109.20
2	B	201	COA	CEP-CBP-CAP	-5.79	98.90	108.77
2	H	201	COA	C5A-C4A-N3A	-5.73	118.83	126.72
2	A	201	COA	CDP-CBP-CCP	5.68	117.59	108.22
2	B	201	COA	N3A-C4A-N9A	5.61	136.71	127.17
2	C	201	COA	N3A-C4A-N9A	5.59	136.68	127.17
2	E	201	COA	C5A-C4A-N3A	-5.55	119.08	126.72
2	H	201	COA	CEP-CBP-CCP	5.52	117.33	108.22
2	G	201	COA	C1B-C2B-C3B	5.36	106.83	101.78
2	K	201	COA	N3A-C4A-N9A	5.25	136.10	127.17
2	F	201	COA	N3A-C4A-N9A	5.21	136.03	127.17
2	D	201	COA	N3A-C4A-N9A	5.21	136.03	127.17
2	B	201	COA	CEP-CBP-CCP	5.18	116.78	108.22
2	A	201	COA	N3A-C4A-N9A	5.10	135.84	127.17
2	K	201	COA	CDP-CBP-CCP	5.01	116.50	108.22
2	C	201	COA	C2A-N3A-C4A	4.98	124.00	111.83
2	J	201	COA	N3A-C4A-N9A	4.98	135.63	127.17
2	H	201	COA	CEP-CBP-CAP	-4.89	100.43	108.77
2	I	201	COA	CDP-CBP-CCP	4.84	116.21	108.22
2	C	201	COA	CEP-CBP-CDP	4.83	118.83	109.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	COA	O6A-CCP-CBP	-4.83	102.78	110.55
2	J	201	COA	C7P-C6P-C5P	4.77	120.33	112.39
2	L	201	COA	C2A-N3A-C4A	4.76	123.46	111.83
2	D	201	COA	C2A-N3A-C4A	4.67	123.22	111.83
2	I	201	COA	N3A-C4A-N9A	4.60	134.99	127.17
2	C	201	COA	C4A-C5A-N7A	-4.55	105.38	110.58
2	J	201	COA	O4B-C1B-N9A	4.54	116.80	108.09
2	H	201	COA	N3A-C4A-N9A	4.53	134.88	127.17
2	E	201	COA	N3A-C4A-N9A	4.52	134.86	127.17
2	B	201	COA	CEP-CBP-CDP	4.52	118.22	109.20
2	A	201	COA	O4B-C1B-N9A	4.45	116.63	108.09
2	I	201	COA	C2A-N3A-C4A	4.36	122.49	111.83
2	I	201	COA	O6A-CCP-CBP	4.34	117.53	110.55
2	C	201	COA	CEP-CBP-CAP	-4.32	101.41	108.77
2	J	201	COA	O6A-CCP-CBP	4.30	117.46	110.55
2	A	201	COA	C2A-N3A-C4A	4.29	122.31	111.83
2	B	201	COA	C2A-N3A-C4A	4.22	122.13	111.83
2	C	201	COA	N3A-C2A-N1A	-4.18	122.26	128.58
2	F	201	COA	C2A-N3A-C4A	4.16	121.98	111.83
2	D	201	COA	N3A-C2A-N1A	-4.14	122.32	128.58
2	K	201	COA	C2A-N3A-C4A	4.12	121.90	111.83
2	B	201	COA	N3A-C2A-N1A	-4.11	122.37	128.58
2	B	201	COA	CAP-C9P-N8P	4.06	118.97	116.32
2	A	201	COA	N3A-C2A-N1A	-4.04	122.47	128.58
2	D	201	COA	C4A-C5A-N7A	-4.00	106.01	110.58
2	I	201	COA	N3A-C2A-N1A	-4.00	122.53	128.58
2	L	201	COA	N3A-C2A-N1A	-3.99	122.54	128.58
2	L	201	COA	C4A-C5A-N7A	-3.99	106.02	110.58
2	K	201	COA	N3A-C2A-N1A	-3.99	122.55	128.58
2	J	201	COA	C2P-C3P-N4P	3.97	121.31	112.31
2	I	201	COA	OAP-CAP-CBP	3.95	116.51	108.73
2	C	201	COA	CEP-CBP-CCP	3.94	114.72	108.22
2	D	201	COA	O6A-CCP-CBP	3.93	116.86	110.55
2	H	201	COA	C2A-N3A-C4A	3.90	121.36	111.83
2	H	201	COA	CEP-CBP-CDP	3.89	116.96	109.20
2	J	201	COA	C2A-N3A-C4A	3.85	121.24	111.83
2	E	201	COA	N3A-C2A-N1A	-3.85	122.75	128.58
2	H	201	COA	N3A-C2A-N1A	-3.84	122.77	128.58
2	E	201	COA	C2A-N3A-C4A	3.84	121.20	111.83
2	I	201	COA	C4A-C5A-N7A	-3.77	106.27	110.58
2	F	201	COA	C4A-C5A-N7A	-3.71	106.34	110.58
2	F	201	COA	N3A-C2A-N1A	-3.67	123.03	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	201	COA	CEP-CBP-CCP	3.63	114.22	108.22
2	C	201	COA	C5A-N7A-C8A	3.58	109.08	103.45
2	J	201	COA	CEP-CBP-CCP	3.57	114.12	108.22
2	J	201	COA	N3A-C2A-N1A	-3.54	123.23	128.58
2	J	201	COA	C4A-C5A-N7A	-3.51	106.56	110.58
2	H	201	COA	C4A-C5A-N7A	-3.51	106.57	110.58
2	E	201	COA	O5P-C5P-C6P	-3.44	115.78	122.02
2	A	201	COA	C4A-C5A-N7A	-3.44	106.65	110.58
2	E	201	COA	CEP-CBP-CDP	3.43	116.04	109.20
2	K	201	COA	C4A-C5A-N7A	-3.36	106.74	110.58
2	E	201	COA	C4A-C5A-N7A	-3.33	106.77	110.58
2	E	201	COA	O6A-CCP-CBP	3.30	115.85	110.55
2	L	201	COA	C2P-C3P-N4P	3.21	119.59	112.31
2	D	201	COA	CEP-CBP-CCP	3.21	113.53	108.22
2	L	201	COA	C5A-N7A-C8A	3.19	108.47	103.45
2	E	201	COA	C3B-C2B-C1B	3.16	106.83	99.89
2	C	201	COA	O6A-CCP-CBP	3.08	115.50	110.55
2	L	201	COA	O4B-C1B-N9A	3.07	113.98	108.09
2	F	201	COA	C5A-N7A-C8A	3.07	108.27	103.45
2	D	201	COA	C5A-N7A-C8A	3.06	108.26	103.45
2	K	201	COA	C3B-C2B-C1B	3.03	106.55	99.89
2	I	201	COA	CBP-CAP-C9P	3.02	118.06	114.70
2	L	201	COA	CEP-CBP-CAP	2.99	113.87	108.77
2	J	201	COA	C5A-N7A-C8A	2.95	108.09	103.45
2	F	201	COA	C3P-N4P-C5P	-2.93	117.37	122.82
2	K	201	COA	O6A-CCP-CBP	2.91	115.23	110.55
2	H	201	COA	C5A-N7A-C8A	2.87	107.96	103.45
2	B	201	COA	C4A-C5A-N7A	-2.82	107.36	110.58
2	F	201	COA	C2P-C3P-N4P	2.79	118.64	112.31
2	H	201	COA	OAP-CAP-CBP	2.76	116.57	110.18
2	H	201	COA	O6A-CCP-CBP	2.73	114.93	110.55
2	B	201	COA	C3B-C2B-C1B	2.71	105.85	99.89
2	E	201	COA	C4A-N9A-C8A	2.69	108.56	105.74
2	E	201	COA	C5A-N7A-C8A	2.68	107.66	103.45
2	H	201	COA	O5B-C5B-C4B	2.68	118.11	108.99
2	H	201	COA	C3B-C2B-C1B	2.64	105.70	99.89
2	I	201	COA	C6A-C5A-N7A	2.63	137.17	132.09
2	B	201	COA	C5A-N7A-C8A	2.63	107.58	103.45
2	I	201	COA	C5A-N7A-C8A	2.60	107.54	103.45
2	D	201	COA	C6A-C5A-N7A	2.60	137.10	132.09
2	J	201	COA	O9A-P3B-O8A	2.60	117.54	107.80
2	A	201	COA	C5A-N7A-C8A	2.59	107.52	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	COA	O4B-C1B-N9A	2.59	113.06	108.09
2	I	201	COA	C3B-C2B-C1B	2.58	105.57	99.89
2	B	201	COA	C4A-N9A-C8A	2.58	108.44	105.74
2	E	201	COA	C2B-C1B-N9A	-2.56	106.94	113.30
2	C	201	COA	O5P-C5P-C6P	-2.52	117.45	122.02
2	H	201	COA	O9A-P3B-O8A	2.50	117.17	107.80
2	G	201	COA	O4B-C4B-C3B	2.49	108.95	104.22
2	A	201	COA	C3B-C2B-C1B	2.49	105.36	99.89
2	F	201	COA	C7P-C6P-C5P	2.49	116.54	112.39
2	I	201	COA	O4B-C1B-N9A	2.48	112.85	108.09
3	H	202	SPM	C12-C11-N10	2.45	118.65	112.07
2	D	201	COA	C2B-C3B-C4B	-2.43	98.98	103.24
2	F	201	COA	C4A-N9A-C8A	2.40	108.26	105.74
2	F	201	COA	O4B-C1B-N9A	2.40	112.70	108.09
2	E	201	COA	C7P-C6P-C5P	-2.40	108.40	112.39
2	D	201	COA	O9P-C9P-N8P	-2.38	119.16	123.13
2	F	201	COA	CEP-CBP-CAP	-2.38	104.71	108.77
2	K	201	COA	C5A-N7A-C8A	2.36	107.16	103.45
2	E	201	COA	CAP-C9P-N8P	2.36	120.96	116.48
2	B	201	COA	O9A-P3B-O8A	2.35	116.63	107.80
2	E	201	COA	C2P-C3P-N4P	-2.35	106.98	112.31
2	C	201	COA	C6A-C5A-N7A	2.34	136.61	132.09
2	J	201	COA	C4A-N9A-C8A	2.33	108.19	105.74
2	A	201	COA	O5B-C5B-C4B	2.32	116.90	108.99
2	E	201	COA	O4B-C1B-N9A	2.31	112.52	108.09
2	K	201	COA	O4B-C1B-N9A	2.30	112.50	108.09
2	H	201	COA	C6A-C5A-N7A	2.28	136.49	132.09
2	L	201	COA	C1B-N9A-C8A	-2.26	122.08	127.09
2	H	201	COA	C4A-N9A-C8A	2.25	108.11	105.74
2	E	201	COA	C6A-C5A-N7A	2.24	136.41	132.09
2	J	201	COA	OAP-CAP-CBP	2.24	115.37	110.18
2	A	201	COA	C2A-N1A-C6A	2.21	122.37	118.73
2	L	201	COA	O4B-C1B-C2B	-2.21	101.89	106.62
2	K	201	COA	C2P-C3P-N4P	-2.21	107.30	112.31
2	E	201	COA	C2A-N1A-C6A	2.20	122.35	118.73
2	L	201	COA	O3B-C3B-C4B	2.20	117.78	110.03
3	J	202	SPM	C12-C11-N10	2.19	117.94	112.07
2	K	201	COA	C2A-N1A-C6A	2.18	122.31	118.73
2	J	201	COA	C2A-N1A-C6A	2.18	122.31	118.73
2	F	201	COA	C6A-C5A-N7A	2.17	136.27	132.09
2	D	201	COA	O4B-C1B-C2B	-2.15	102.03	106.62
2	I	201	COA	C2A-N1A-C6A	2.14	122.24	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	COA	O4B-C1B-C2B	-2.13	102.05	106.62
2	E	201	COA	N9A-C8A-N7A	-2.12	110.93	113.94
2	E	201	COA	O3A-P1A-O1A	-2.11	104.34	110.70
2	L	201	COA	C6A-C5A-N7A	2.11	136.16	132.09
2	H	201	COA	C2A-N1A-C6A	2.11	122.20	118.73
2	K	201	COA	O5A-P2A-O4A	2.10	122.22	112.44
2	F	201	COA	N9A-C8A-N7A	-2.10	110.96	113.94
2	A	201	COA	C2B-C3B-C4B	2.08	106.88	103.24
2	C	201	COA	O5A-P2A-O4A	2.07	122.10	112.44
2	B	201	COA	C2A-N1A-C6A	2.05	122.11	118.73
2	A	201	COA	C6A-C5A-N7A	2.04	136.03	132.09
2	B	201	COA	C1B-N9A-C8A	-2.04	122.56	127.09
2	D	201	COA	O3B-C3B-C4B	2.04	117.22	110.03
2	J	201	COA	O5A-P2A-O3A	2.04	112.79	107.27
2	K	201	COA	O5P-C5P-C6P	-2.03	118.34	122.02
2	E	201	COA	O5P-C5P-N4P	2.02	127.00	123.03
2	J	201	COA	P3B-O3B-C3B	-2.02	118.04	123.43
2	H	201	COA	N9A-C8A-N7A	-2.02	111.07	113.94
2	J	201	COA	N9A-C8A-N7A	-2.02	111.08	113.94
2	K	201	COA	O9A-P3B-O8A	2.01	115.33	107.80

There are no chirality outliers.

All (202) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	COA	CDP-CBP-CCP-O6A
2	A	201	COA	CEP-CBP-CCP-O6A
2	A	201	COA	CAP-CBP-CCP-O6A
2	B	201	COA	CEP-CBP-CCP-O6A
2	C	201	COA	CCP-O6A-P2A-O3A
2	C	201	COA	C9P-CAP-CBP-CCP
2	C	201	COA	C9P-CAP-CBP-CDP
2	C	201	COA	OAP-CAP-CBP-CEP
2	C	201	COA	C9P-CAP-CBP-CEP
2	C	201	COA	C5P-C6P-C7P-N8P
2	D	201	COA	C2B-C1B-N9A-C4A
2	D	201	COA	C3B-C4B-C5B-O5B
2	D	201	COA	O4B-C4B-C5B-O5B
2	D	201	COA	C5B-O5B-P1A-O2A
2	D	201	COA	C5B-O5B-P1A-O3A
2	D	201	COA	CEP-CBP-CCP-O6A
2	D	201	COA	CAP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
2	D	201	COA	O9P-C9P-CAP-CBP
2	D	201	COA	N8P-C9P-CAP-OAP
2	E	201	COA	CDP-CBP-CCP-O6A
2	E	201	COA	C5P-C6P-C7P-N8P
2	F	201	COA	O4B-C1B-N9A-C4A
2	F	201	COA	O4B-C1B-N9A-C8A
2	F	201	COA	C5B-O5B-P1A-O1A
2	F	201	COA	C5B-O5B-P1A-O3A
2	F	201	COA	CEP-CBP-CCP-O6A
2	F	201	COA	CAP-CBP-CCP-O6A
2	G	201	COA	P1A-O3A-P2A-O5A
2	H	201	COA	C5B-O5B-P1A-O2A
2	H	201	COA	CDP-CBP-CCP-O6A
2	H	201	COA	N8P-C9P-CAP-OAP
2	I	201	COA	CCP-O6A-P2A-O3A
2	I	201	COA	CDP-CBP-CCP-O6A
2	I	201	COA	CAP-CBP-CCP-O6A
2	I	201	COA	C9P-CAP-CBP-CEP
2	J	201	COA	C5B-O5B-P1A-O1A
2	J	201	COA	C5B-O5B-P1A-O3A
2	J	201	COA	CDP-CBP-CCP-O6A
2	J	201	COA	N8P-C9P-CAP-OAP
2	K	201	COA	CEP-CBP-CCP-O6A
2	K	201	COA	CAP-CBP-CCP-O6A
2	K	201	COA	C5P-C6P-C7P-N8P
2	L	201	COA	O4B-C4B-C5B-O5B
2	L	201	COA	C5B-O5B-P1A-O2A
2	L	201	COA	C5B-O5B-P1A-O3A
2	L	201	COA	CDP-CBP-CCP-O6A
2	L	201	COA	CEP-CBP-CCP-O6A
2	L	201	COA	CAP-CBP-CCP-O6A
2	L	201	COA	C9P-CAP-CBP-CCP
2	L	201	COA	C9P-CAP-CBP-CDP
2	L	201	COA	C9P-CAP-CBP-CEP
2	L	201	COA	C5P-C6P-C7P-N8P
2	L	201	COA	C2P-C3P-N4P-C5P
2	L	201	COA	S1P-C2P-C3P-N4P
3	G	202	SPM	C3-C4-N5-C6
3	I	202	SPM	C3-C4-N5-C6
2	J	201	COA	C6P-C5P-N4P-C3P
2	F	201	COA	C3B-C4B-C5B-O5B
2	J	201	COA	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	F	201	COA	C6P-C5P-N4P-C3P
3	J	202	SPM	C7-C8-C9-N10
3	J	202	SPM	N5-C6-C7-C8
2	D	201	COA	C2B-C1B-N9A-C8A
3	G	202	SPM	N10-C11-C12-C13
3	I	202	SPM	N10-C11-C12-C13
3	K	202	SPM	C2-C3-C4-N5
3	H	202	SPM	C2-C3-C4-N5
3	E	202	SPM	C7-C8-C9-N10
2	C	201	COA	O4B-C4B-C5B-O5B
2	F	201	COA	O4B-C4B-C5B-O5B
2	H	201	COA	C3B-C4B-C5B-O5B
2	H	201	COA	O4B-C4B-C5B-O5B
2	K	201	COA	O4B-C4B-C5B-O5B
2	L	201	COA	C3B-C4B-C5B-O5B
2	J	201	COA	O4B-C1B-N9A-C4A
4	L	202	PEG	O2-C3-C4-O4
2	L	201	COA	C2B-C1B-N9A-C4A
3	E	202	SPM	N5-C6-C7-C8
3	H	202	SPM	C7-C8-C9-N10
2	A	201	COA	C2B-C3B-O3B-P3B
2	E	201	COA	C2B-C3B-O3B-P3B
3	J	202	SPM	N10-C11-C12-C13
3	I	202	SPM	C8-C9-N10-C11
2	C	201	COA	C3B-C4B-C5B-O5B
2	K	201	COA	C3B-C4B-C5B-O5B
2	H	201	COA	C6P-C7P-N8P-C9P
2	J	201	COA	O5P-C5P-N4P-C3P
3	I	202	SPM	N5-C6-C7-C8
2	F	201	COA	C6P-C7P-N8P-C9P
3	E	202	SPM	C7-C6-N5-C4
3	K	202	SPM	C7-C6-N5-C4
2	J	201	COA	O4B-C4B-C5B-O5B
2	A	201	COA	C4B-C3B-O3B-P3B
2	H	201	COA	C2B-C3B-O3B-P3B
2	C	201	COA	C2B-C1B-N9A-C8A
2	L	201	COA	C2B-C1B-N9A-C8A
4	H	203	PEG	O1-C1-C2-O2
2	C	201	COA	C2B-C1B-N9A-C4A
3	K	202	SPM	N1-C2-C3-C4
2	F	201	COA	O5P-C5P-N4P-C3P
2	E	201	COA	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	E	202	SPM	C2-C3-C4-N5
2	B	201	COA	C2B-C3B-O3B-P3B
4	H	203	PEG	O2-C3-C4-O4
2	D	201	COA	O9P-C9P-CAP-OAP
3	H	202	SPM	N5-C6-C7-C8
2	C	201	COA	OAP-CAP-CBP-CDP
2	L	201	COA	OAP-CAP-CBP-CDP
3	J	202	SPM	C6-C7-C8-C9
2	B	201	COA	O4B-C4B-C5B-O5B
2	L	201	COA	N8P-C9P-CAP-CBP
3	H	202	SPM	C6-C7-C8-C9
3	I	202	SPM	C6-C7-C8-C9
2	B	201	COA	N8P-C9P-CAP-OAP
3	G	202	SPM	C6-C7-C8-C9
2	E	201	COA	C3B-C4B-C5B-O5B
3	E	202	SPM	N1-C2-C3-C4
3	G	202	SPM	N1-C2-C3-C4
3	H	202	SPM	C8-C9-N10-C11
2	C	201	COA	C2B-C3B-O3B-P3B
2	F	201	COA	C5P-C6P-C7P-N8P
4	I	203	PEG	O2-C3-C4-O4
3	G	202	SPM	C8-C9-N10-C11
2	J	201	COA	O4B-C1B-N9A-C8A
2	C	201	COA	P2A-O3A-P1A-O1A
2	J	201	COA	P1A-O3A-P2A-O4A
2	K	201	COA	P2A-O3A-P1A-O1A
2	B	201	COA	O9P-C9P-CAP-OAP
2	E	201	COA	O9P-C9P-CAP-OAP
2	H	201	COA	O9P-C9P-CAP-OAP
2	J	201	COA	O9P-C9P-CAP-OAP
2	C	201	COA	CDP-CBP-CCP-O6A
2	C	201	COA	CEP-CBP-CCP-O6A
2	E	201	COA	CEP-CBP-CCP-O6A
2	F	201	COA	CDP-CBP-CCP-O6A
2	I	201	COA	CEP-CBP-CCP-O6A
2	C	201	COA	S1P-C2P-C3P-N4P
2	E	201	COA	S1P-C2P-C3P-N4P
2	F	201	COA	S1P-C2P-C3P-N4P
2	H	201	COA	S1P-C2P-C3P-N4P
2	B	201	COA	C2B-C1B-N9A-C4A
2	C	201	COA	CCP-O6A-P2A-O4A
2	C	201	COA	CCP-O6A-P2A-O5A

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Mol	Chain	Res	Type	Atoms
2	C	201	COA	OAP-CAP-CBP-CCP
2	D	201	COA	C5B-O5B-P1A-O1A
2	F	201	COA	C5B-O5B-P1A-O2A
2	H	201	COA	C5B-O5B-P1A-O1A
2	H	201	COA	C5B-O5B-P1A-O3A
2	I	201	COA	CCP-O6A-P2A-O4A
2	J	201	COA	C5B-O5B-P1A-O2A
2	L	201	COA	C5B-O5B-P1A-O1A
3	E	202	SPM	C6-C7-C8-C9
2	B	201	COA	C2B-C1B-N9A-C8A
3	E	202	SPM	C11-C12-C13-N14
3	G	202	SPM	C7-C6-N5-C4
3	J	202	SPM	C3-C4-N5-C6
3	J	202	SPM	C11-C12-C13-N14
2	B	201	COA	C3B-C4B-C5B-O5B
2	L	201	COA	O9P-C9P-CAP-CBP
3	I	202	SPM	C12-C11-N10-C9
2	G	201	COA	C3B-O3B-P3B-O9A
2	G	201	COA	C4B-C5B-O5B-P1A
2	D	201	COA	N8P-C9P-CAP-CBP
2	I	201	COA	OAP-CAP-CBP-CDP
3	I	202	SPM	C7-C6-N5-C4
2	E	201	COA	N8P-C9P-CAP-OAP
2	G	201	COA	O4B-C4B-C5B-O5B
2	C	201	COA	C3B-O3B-P3B-O7A
2	E	201	COA	C3B-O3B-P3B-O7A
2	J	201	COA	C3B-O3B-P3B-O7A
3	E	202	SPM	N10-C11-C12-C13
2	K	201	COA	O4B-C1B-N9A-C8A
2	G	201	COA	P1A-O3A-P2A-O6A
2	B	201	COA	C4B-C3B-O3B-P3B
2	H	201	COA	C4B-C3B-O3B-P3B
3	H	202	SPM	C12-C11-N10-C9
2	F	201	COA	C9P-CAP-CBP-CEP
2	B	201	COA	O4B-C1B-N9A-C8A
4	I	203	PEG	O1-C1-C2-O2
3	E	202	SPM	C12-C11-N10-C9
3	J	202	SPM	C8-C9-N10-C11
2	L	201	COA	OAP-CAP-CBP-CEP
2	E	201	COA	P2A-O3A-P1A-O2A
2	F	201	COA	P2A-O3A-P1A-O2A
2	K	201	COA	P2A-O3A-P1A-O2A

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Mol	Chain	Res	Type	Atoms
2	L	201	COA	P1A-O3A-P2A-O5A
2	C	201	COA	C3B-O3B-P3B-O9A
2	E	201	COA	C3B-O3B-P3B-O8A
2	J	201	COA	C3B-O3B-P3B-O9A
2	E	201	COA	C4B-C3B-O3B-P3B
2	K	201	COA	C2B-C1B-N9A-C4A
2	G	201	COA	P1A-O3A-P2A-O4A
3	I	202	SPM	C11-C12-C13-N14
2	I	201	COA	O4B-C1B-N9A-C8A
2	I	201	COA	C3B-O3B-P3B-O7A
2	K	201	COA	C2B-C1B-N9A-C8A
3	H	202	SPM	C3-C4-N5-C6
3	K	202	SPM	C8-C9-N10-C11
2	B	201	COA	P1A-O3A-P2A-O5A
2	C	201	COA	P2A-O3A-P1A-O2A
2	D	201	COA	P2A-O3A-P1A-O2A
2	H	201	COA	P1A-O3A-P2A-O5A

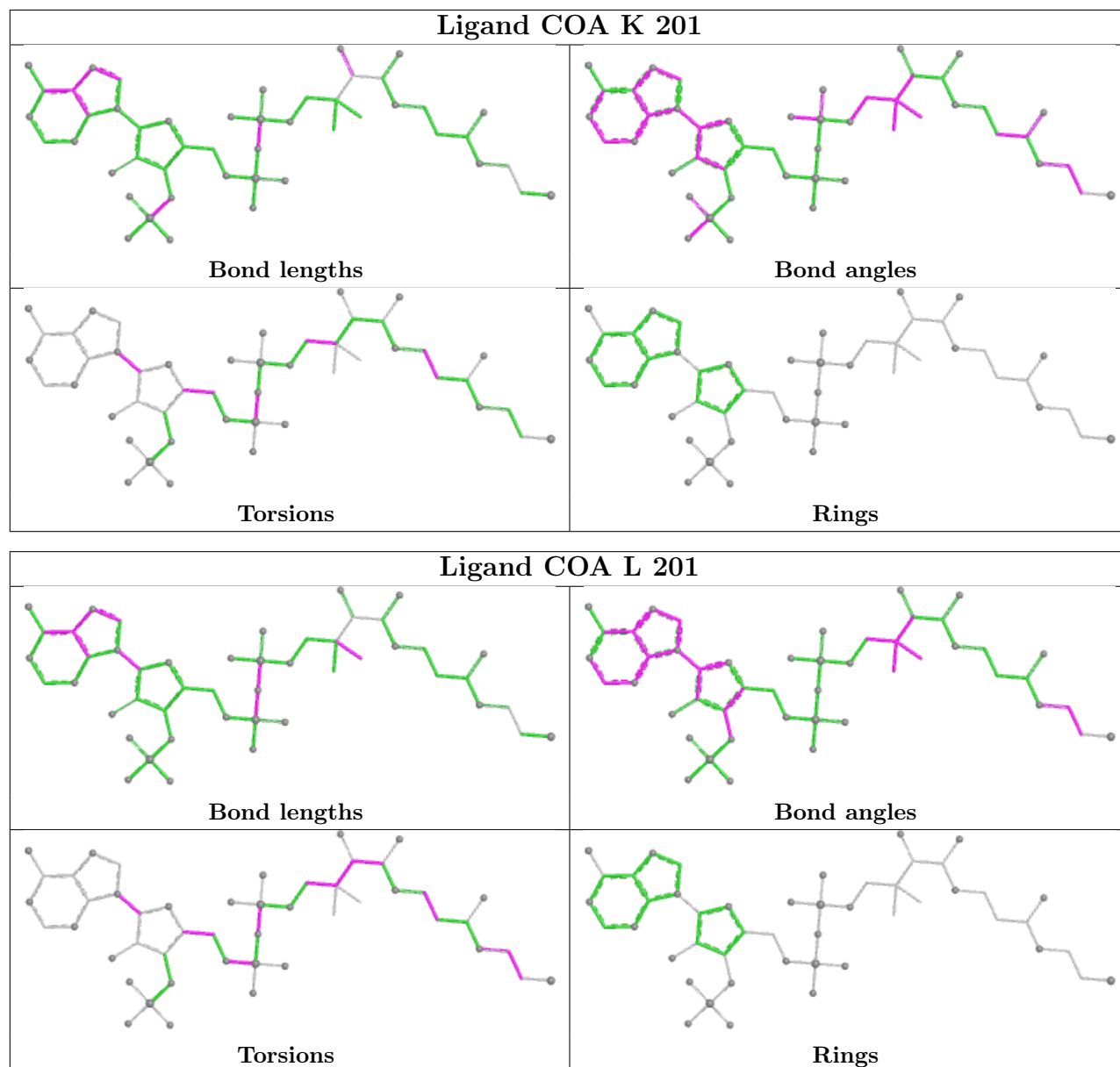
There are no ring outliers.

12 monomers are involved in 28 short contacts:

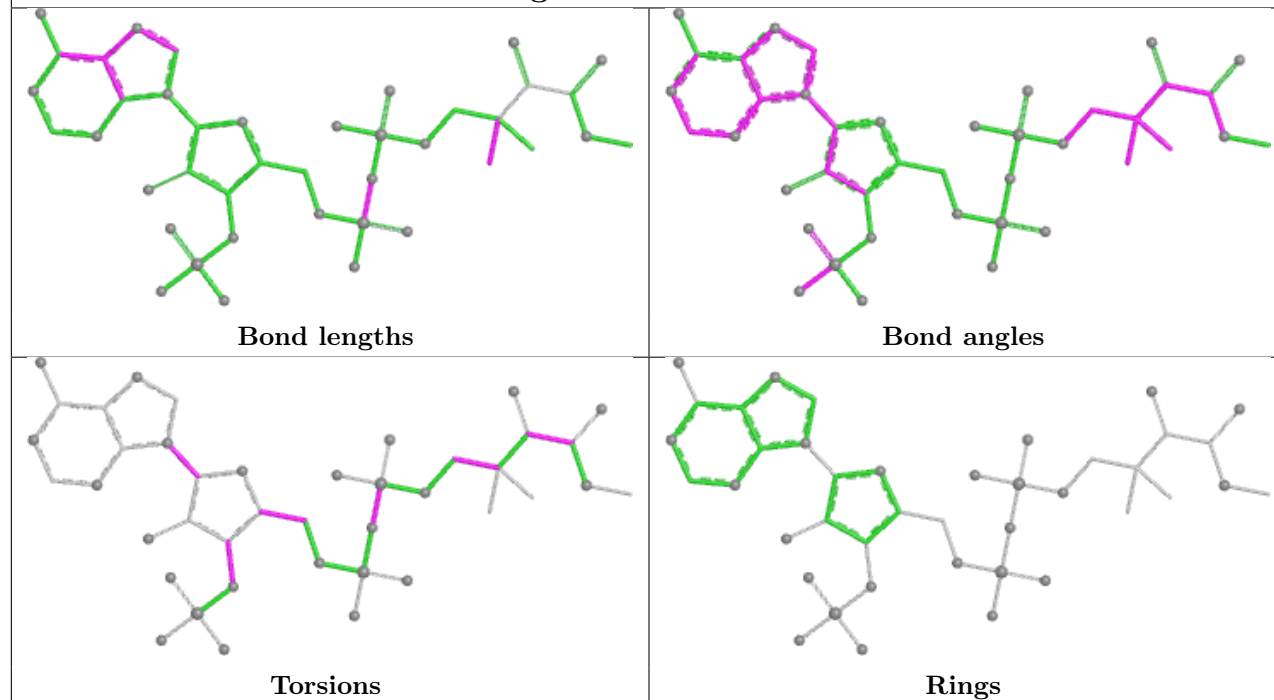
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	201	COA	1	0
2	L	201	COA	6	0
2	B	201	COA	3	0
3	K	202	SPM	1	0
2	G	201	COA	1	0
2	H	201	COA	1	0
3	E	202	SPM	1	0
2	C	201	COA	3	0
2	E	201	COA	2	0
2	F	201	COA	3	0
2	J	201	COA	5	0
3	J	202	SPM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

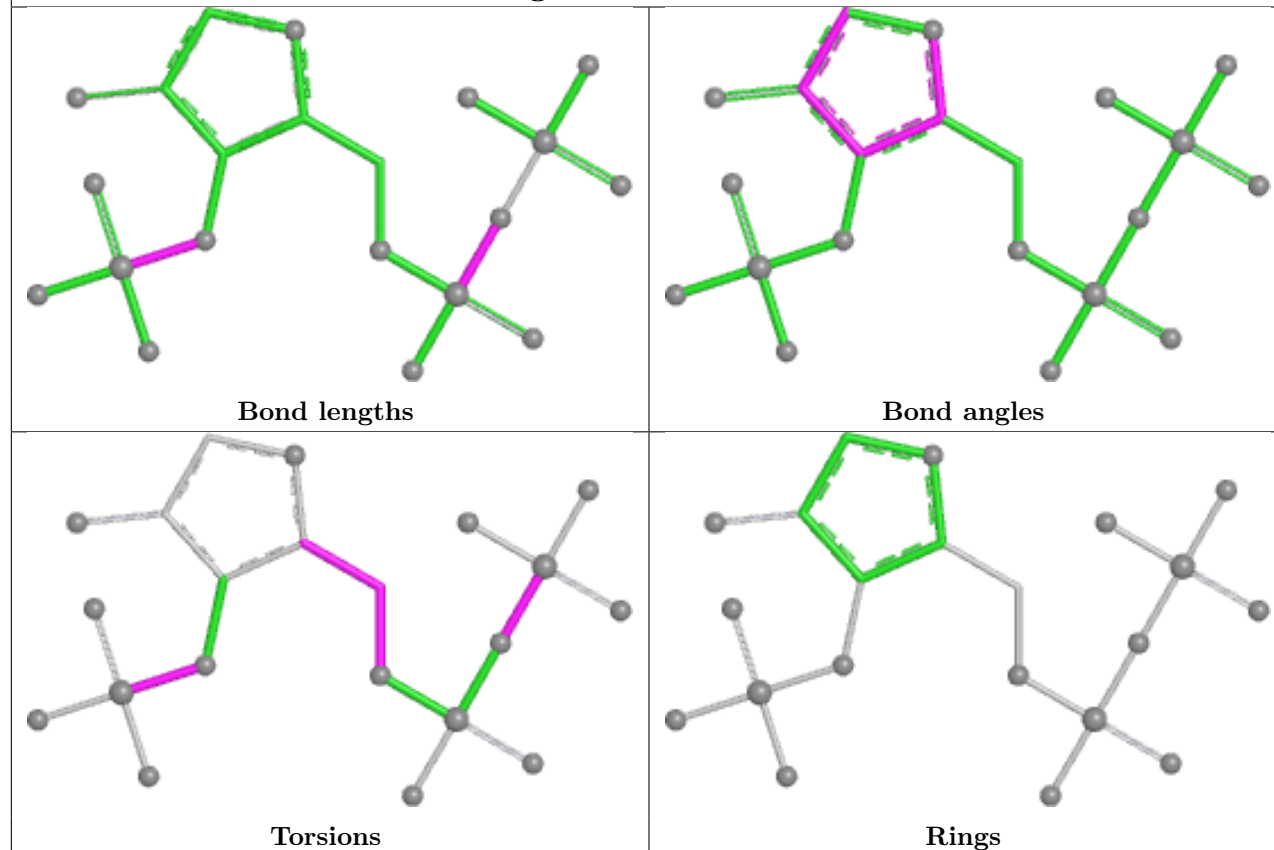
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

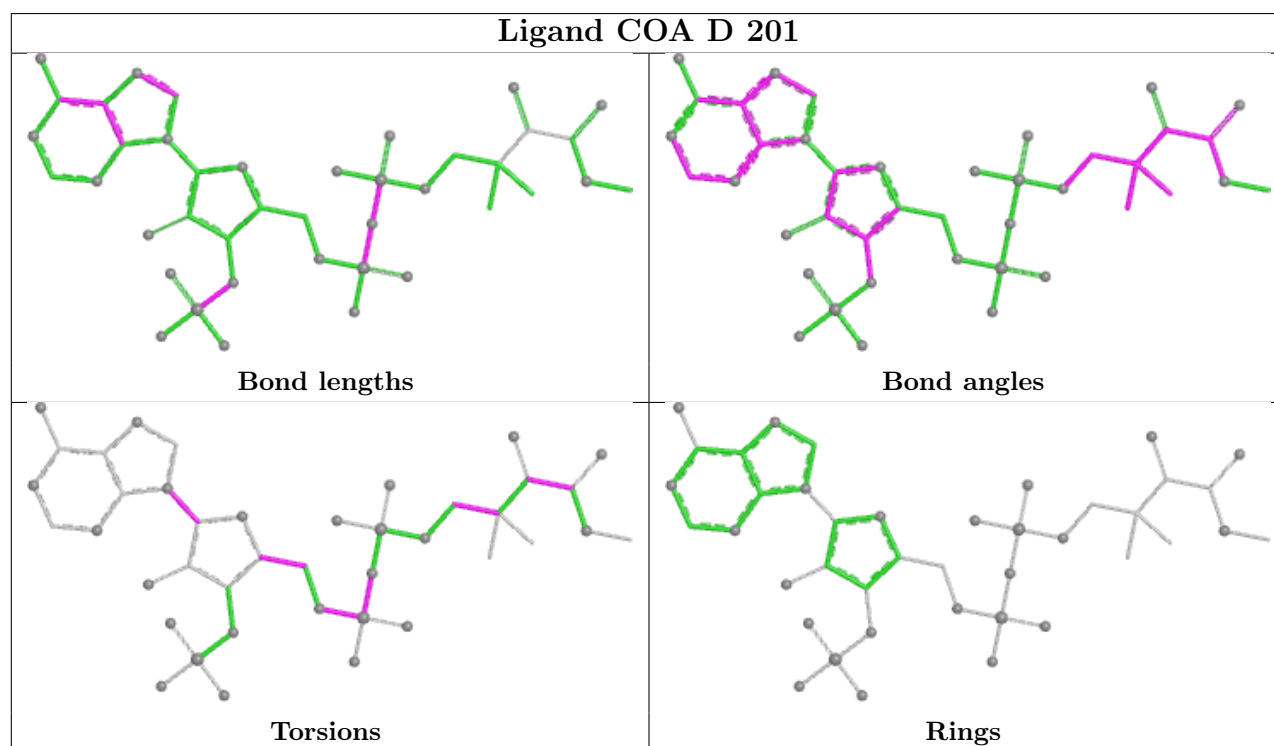
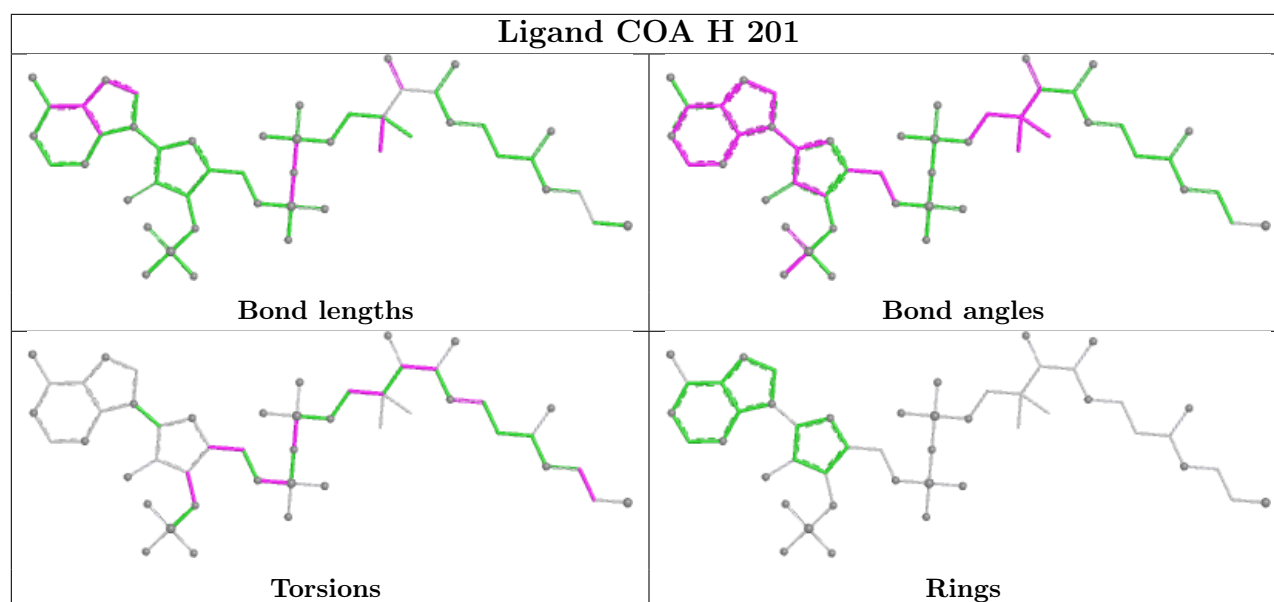


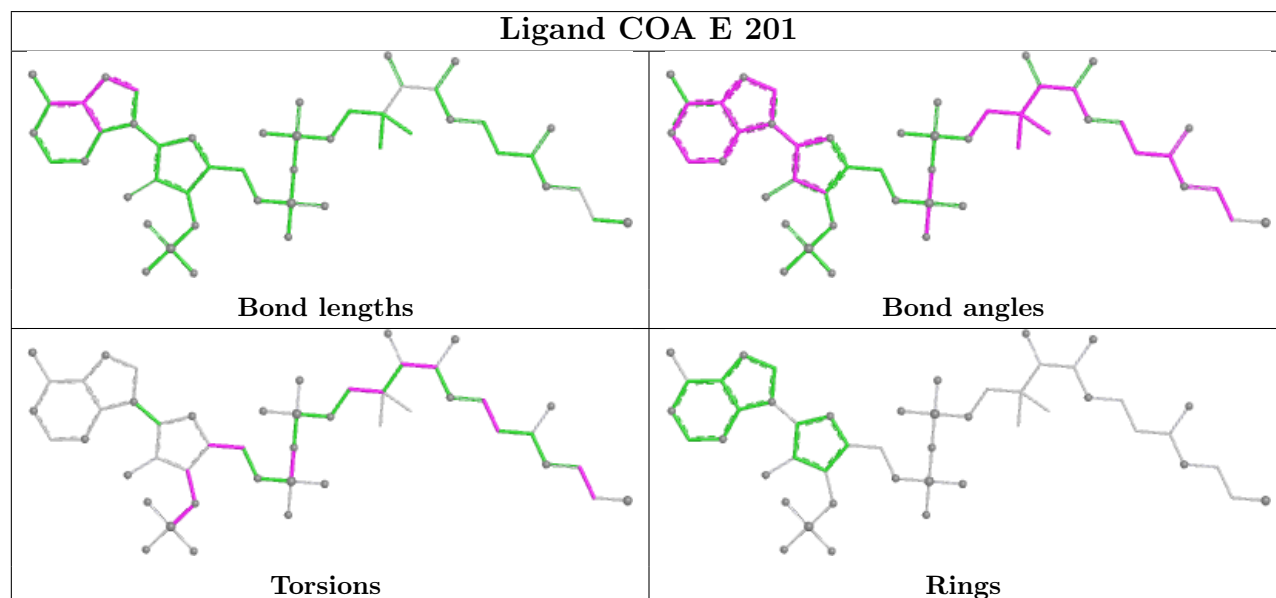
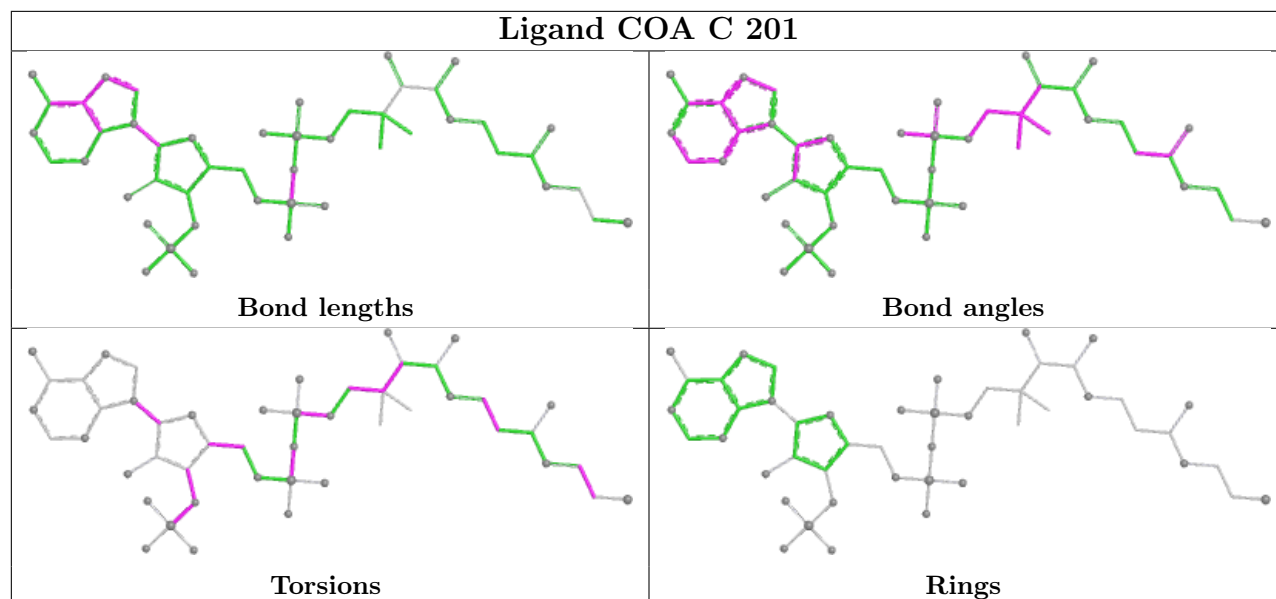
Ligand COA B 201

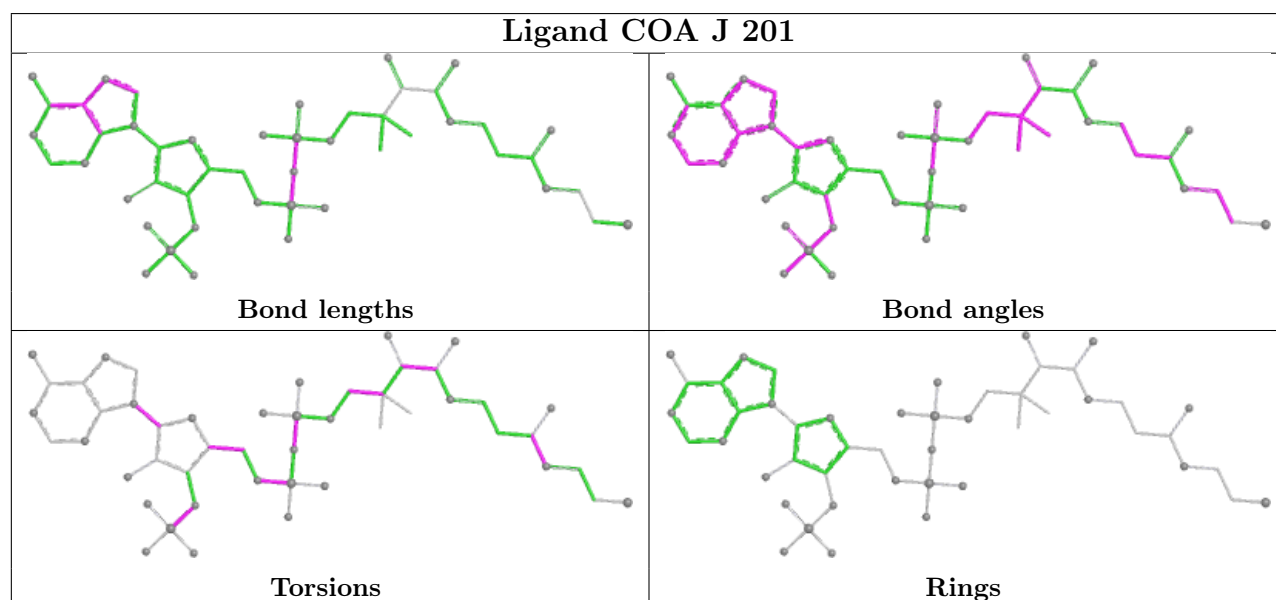
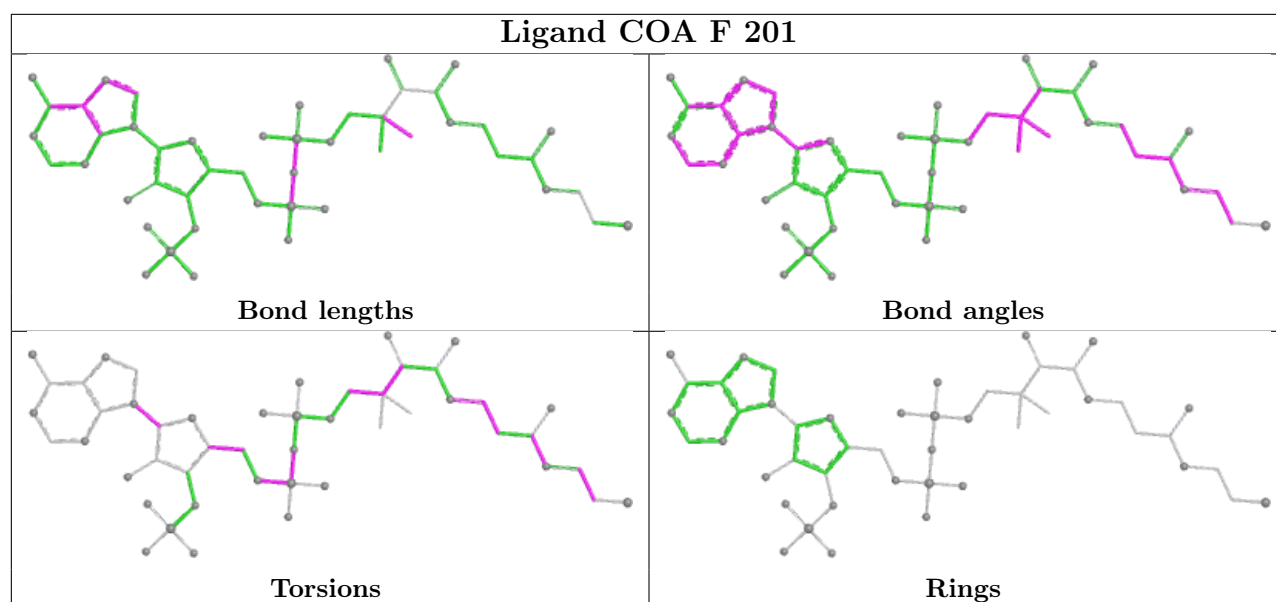


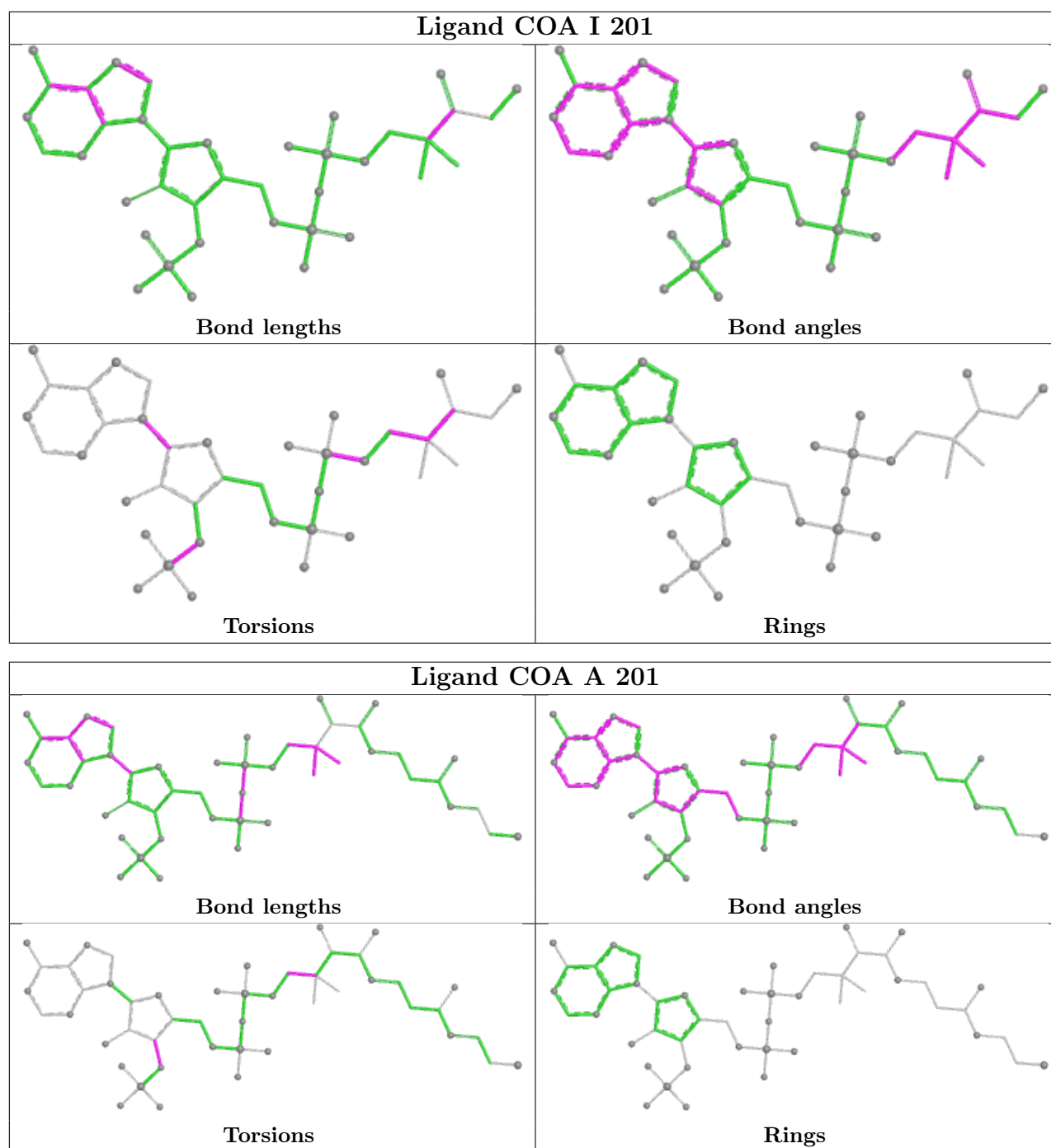
Ligand COA G 201











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	170/176 (96%)	-0.60	0 100 100	25, 41, 58, 70	0
1	B	169/176 (96%)	-0.67	0 100 100	19, 37, 55, 76	1 (0%)
1	C	169/176 (96%)	-0.64	0 100 100	28, 38, 55, 60	0
1	D	168/176 (95%)	-0.58	0 100 100	29, 40, 61, 74	0
1	E	170/176 (96%)	-0.85	0 100 100	20, 31, 47, 55	0
1	F	169/176 (96%)	-0.85	1 (0%) 85 83	20, 32, 47, 75	0
1	G	170/176 (96%)	-0.78	0 100 100	18, 32, 50, 79	1 (0%)
1	H	169/176 (96%)	-0.85	0 100 100	21, 30, 47, 72	0
1	I	169/176 (96%)	-0.75	0 100 100	25, 36, 46, 60	0
1	J	169/176 (96%)	-0.69	0 100 100	16, 37, 48, 66	1 (0%)
1	K	170/176 (96%)	-0.65	0 100 100	22, 38, 59, 70	0
1	L	169/176 (96%)	-0.70	0 100 100	24, 37, 51, 58	0
All	All	2031/2112 (96%)	-0.72	1 (0%) 100 100	16, 36, 54, 79	3 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	83	ALA	2.6

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

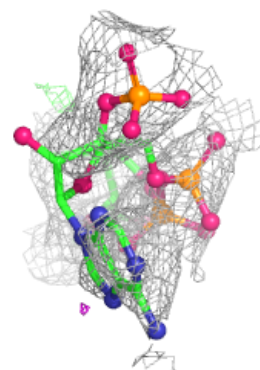
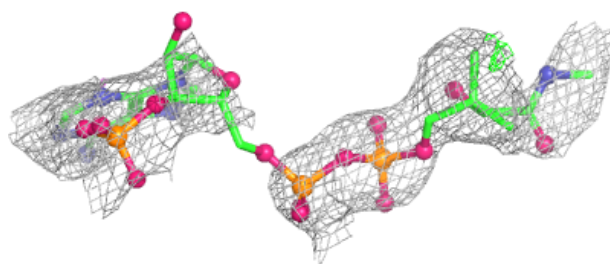
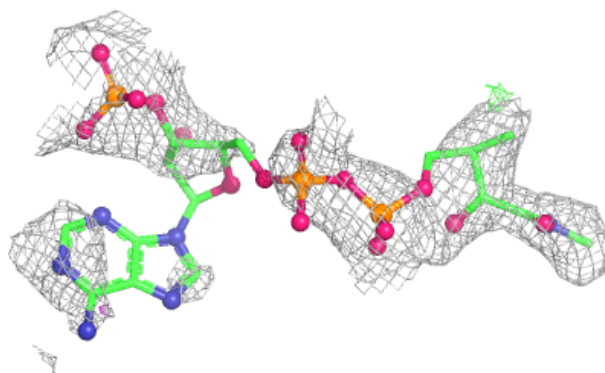
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	COA	D	201	41/48	0.94	0.12	39,86,101,102	0
2	COA	G	201	21/48	0.94	0.12	90,98,102,106	0
2	COA	I	201	39/48	0.94	0.11	45,80,90,91	0
2	COA	A	201	48/48	0.95	0.09	49,68,85,93	0
2	COA	L	201	48/48	0.95	0.10	45,62,105,108	0
2	COA	F	201	48/48	0.96	0.08	46,59,97,99	0
2	COA	K	201	48/48	0.96	0.09	44,58,92,96	0
2	COA	C	201	48/48	0.96	0.08	45,61,88,94	0
3	SPM	I	202	14/14	0.96	0.10	34,39,42,42	0
4	PEG	I	203	7/7	0.96	0.09	56,58,60,62	0
3	SPM	E	202	14/14	0.97	0.07	34,39,40,42	0
3	SPM	H	202	14/14	0.97	0.09	39,45,49,51	0
2	COA	B	201	41/48	0.97	0.09	39,54,72,75	0
3	SPM	J	202	14/14	0.97	0.09	26,34,47,50	0
3	SPM	K	202	14/14	0.97	0.07	39,42,45,45	0
4	PEG	H	203	7/7	0.97	0.07	38,40,45,47	0
2	COA	J	201	48/48	0.97	0.08	33,46,85,87	0
4	PEG	L	202	7/7	0.97	0.08	45,45,47,48	0
2	COA	E	201	48/48	0.98	0.07	34,50,97,105	0
3	SPM	G	202	14/14	0.98	0.07	28,32,34,37	0
2	COA	H	201	48/48	0.98	0.07	38,50,59,60	0

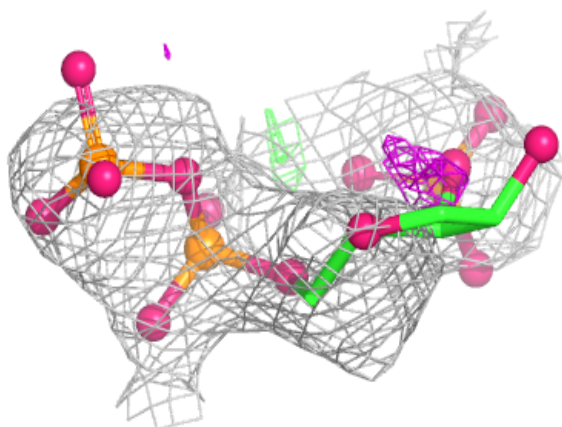
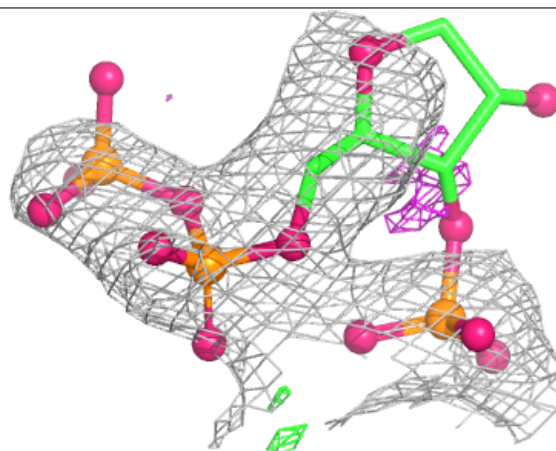
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA D 201:

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

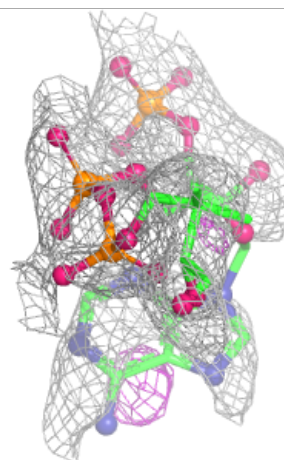
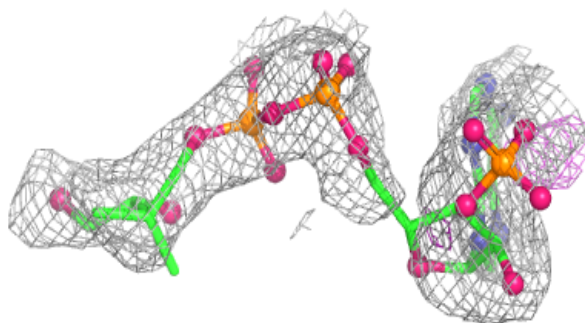
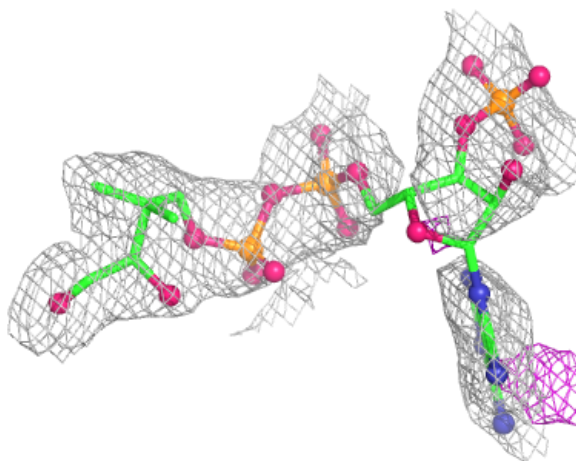
**Electron density around COA G 201:**

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



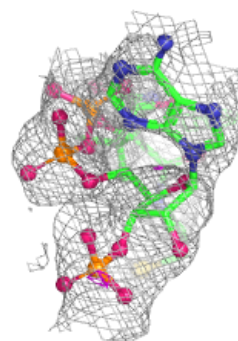
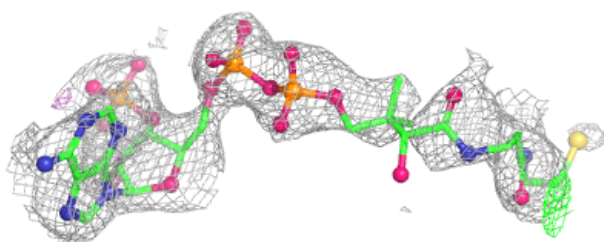
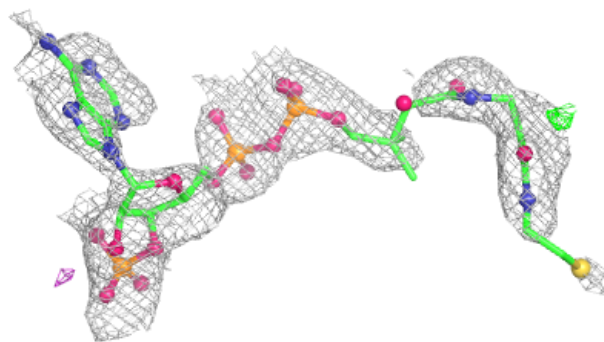
Electron density around COA I 201:

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

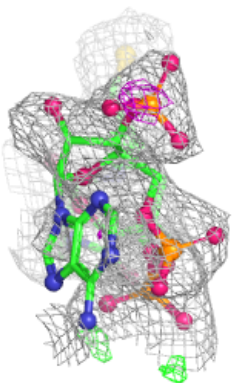
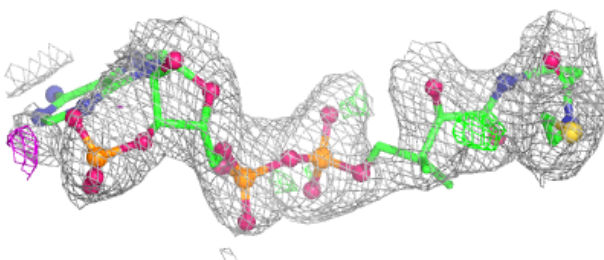
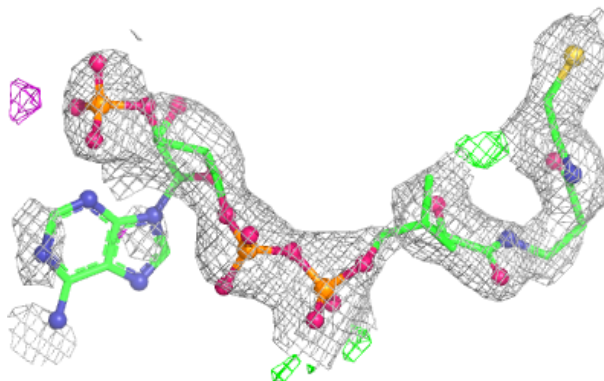


Electron density around COA A 201:

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

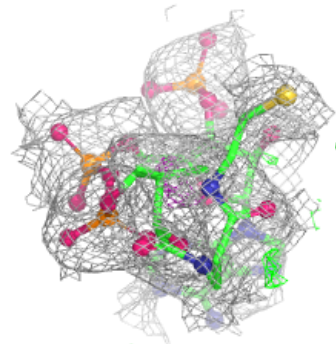
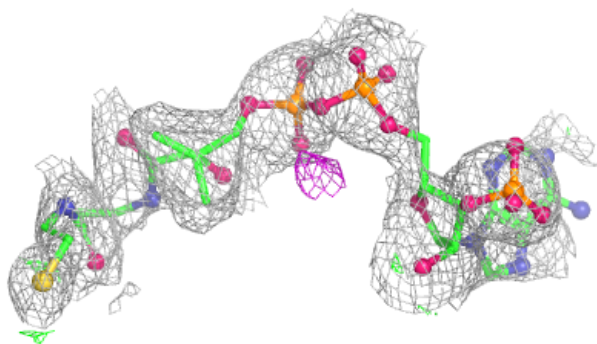
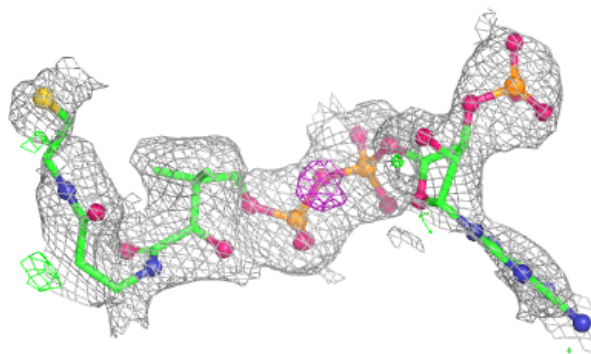
**Electron density around COA L 201:**

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and green (positive)

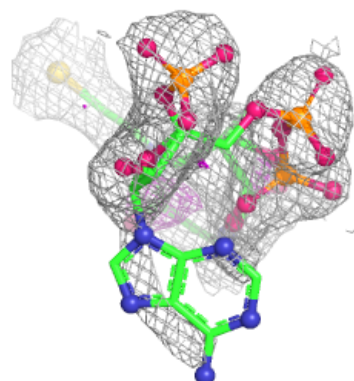
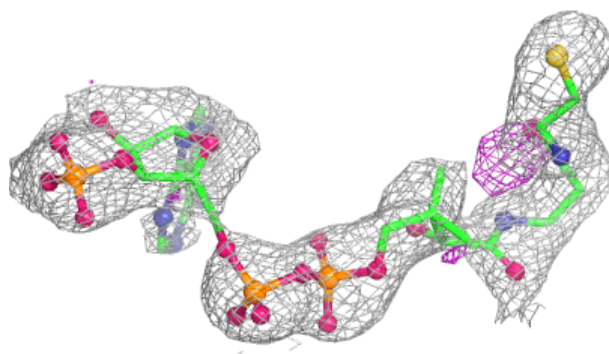
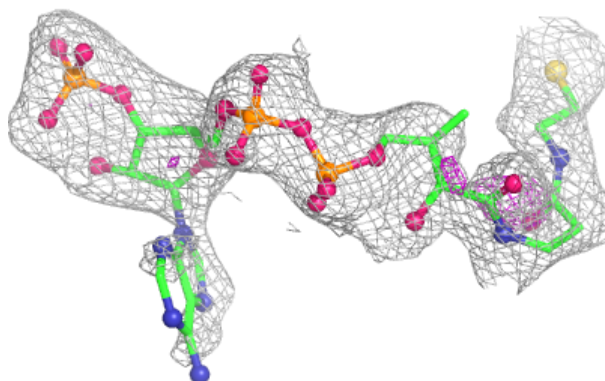


Electron density around COA F 201:

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

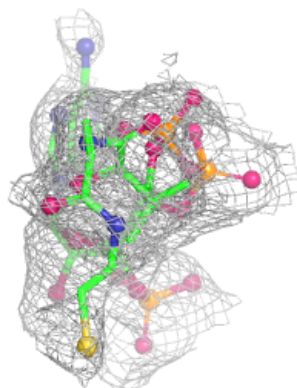
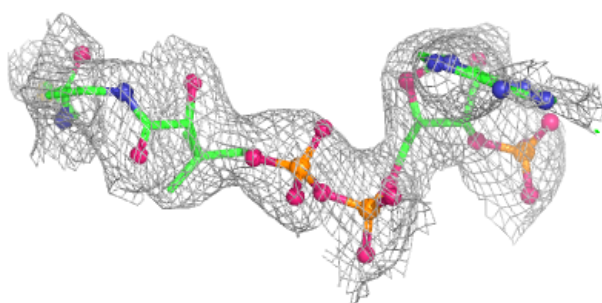
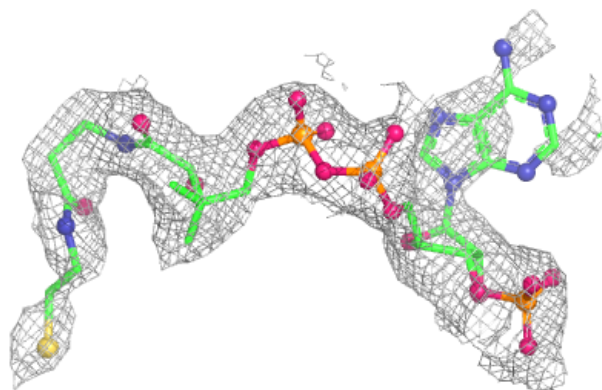
**Electron density around COA K 201:**

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and green (positive)

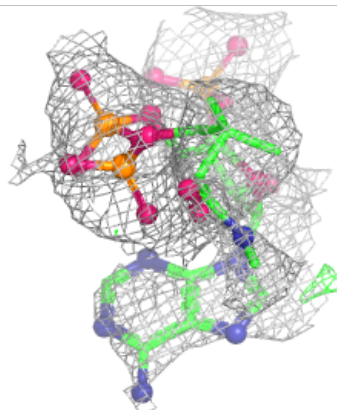
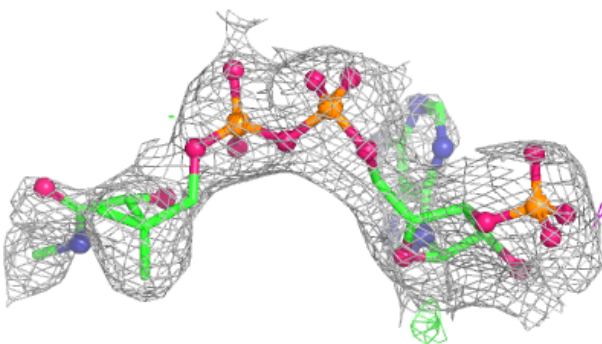
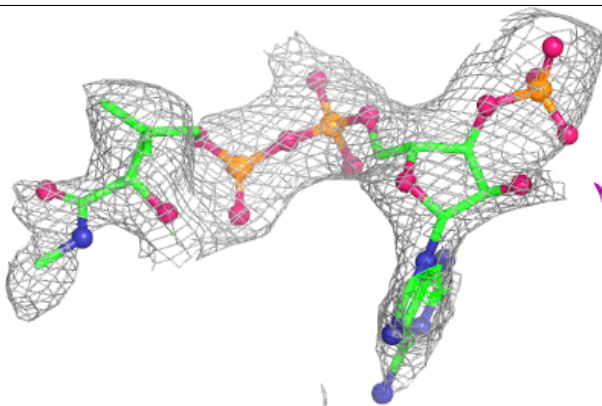


Electron density around COA C 201:

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and green (positive)

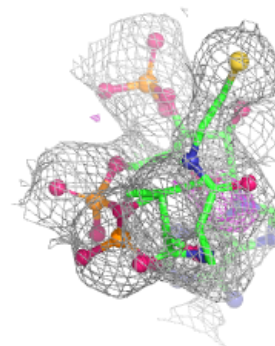
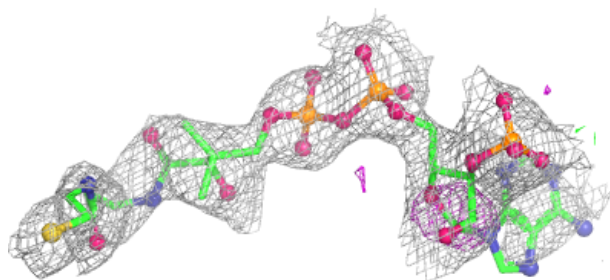
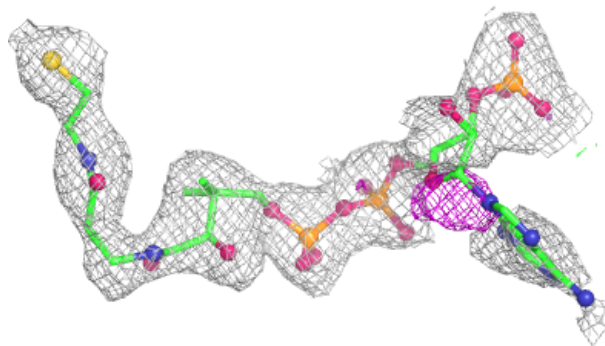
**Electron density around COA B 201:**

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

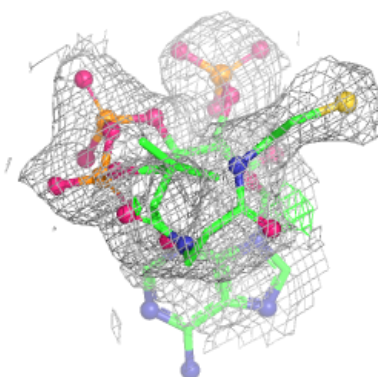
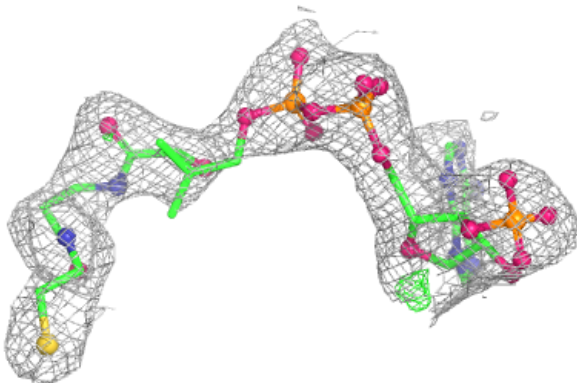
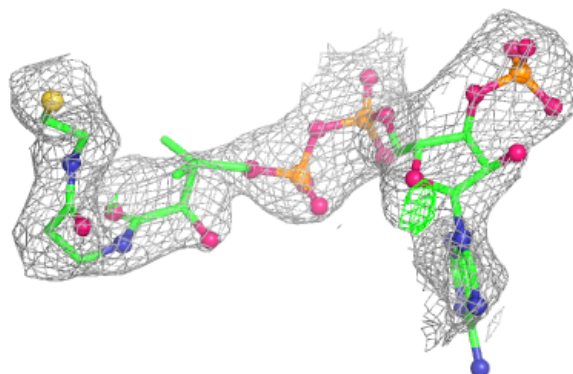


Electron density around COA J 201:

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

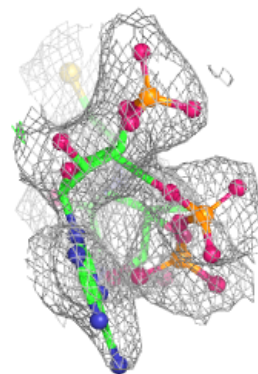
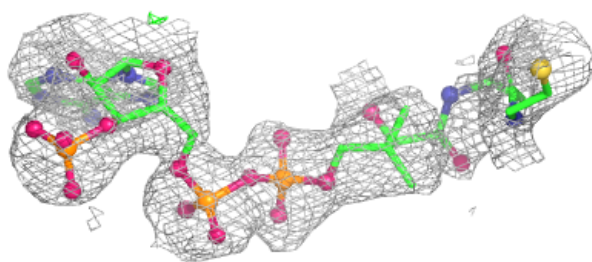
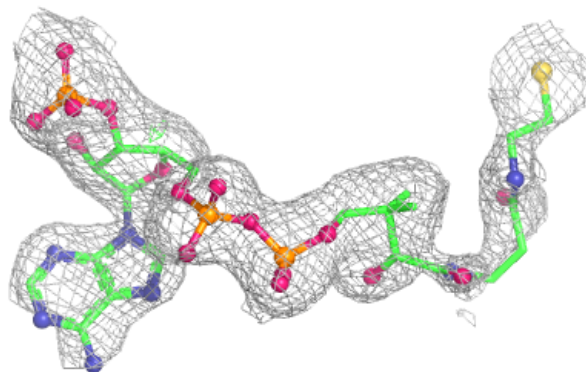
**Electron density around COA E 201:**

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



Electron density around COA H 201:

$2mF_o-DF_c$ (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.