



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:55 AM UTC

PDB ID : 8GXF / pdb_00008gxf
Title : Pseudomonas flexibilis GCN5 family acetyltransferase
Authors : Song, Y.J.; Bao, R.
Deposited on : 2022-09-20
Resolution : 3.04 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

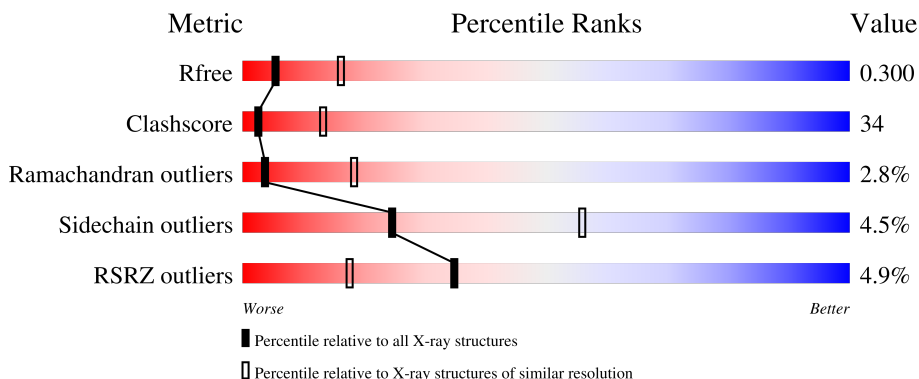
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	193	 4% 41% 45% 10% ..
1	B	193	 6% 47% 39% 8% ..
1	C	193	 3% 42% 45% 8% ..
1	D	193	 7% 53% 38% 5% ..

2 Entry composition i

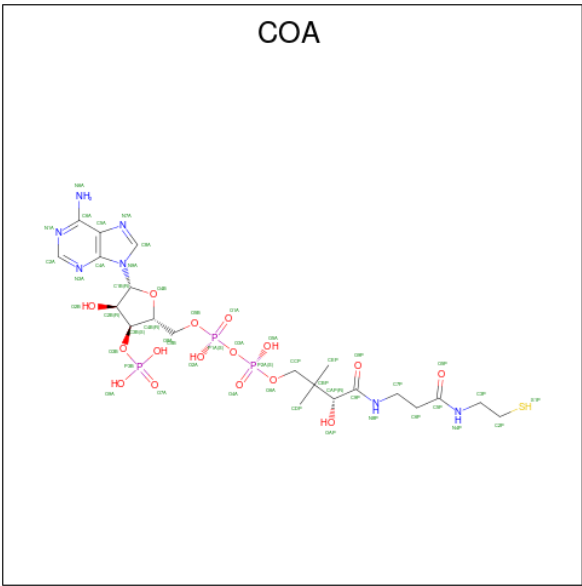
There are 3 unique types of molecules in this entry. The entry contains 6245 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GCN5 family acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	187	Total	C	N	O	S	0	0	0
			1504	944	283	272	5			
1	A	187	Total	C	N	O	S	0	0	0
			1504	944	283	272	5			
1	C	187	Total	C	N	O	S	0	0	0
			1504	944	283	272	5			
1	D	187	Total	C	N	O	S	0	0	0
			1504	944	283	272	5			

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S) (labeled as "Ligand of Interest" by depositor).



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

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

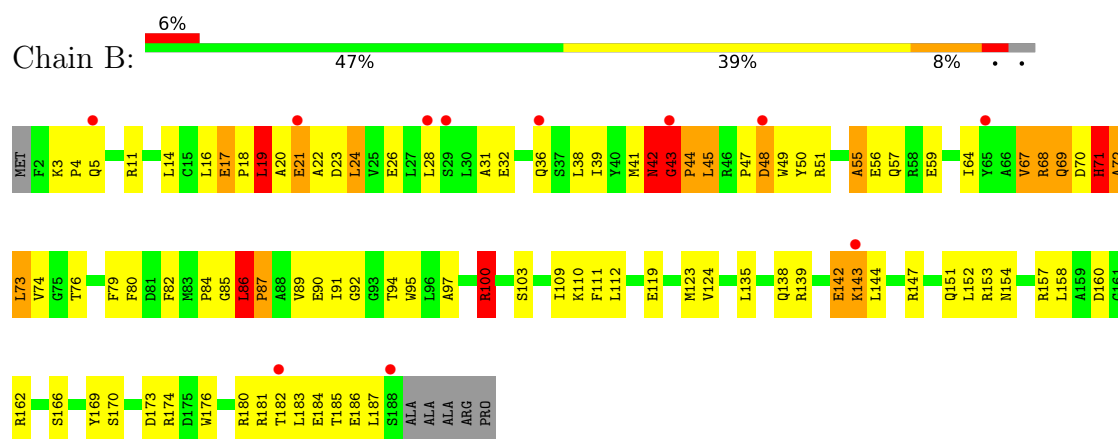
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	6	Total	O	0	0
			6	6		
3	A	13	Total	O	0	0
			13	13		
3	C	11	Total	O	0	0
			11	11		
3	D	7	Total	O	0	0
			7	7		

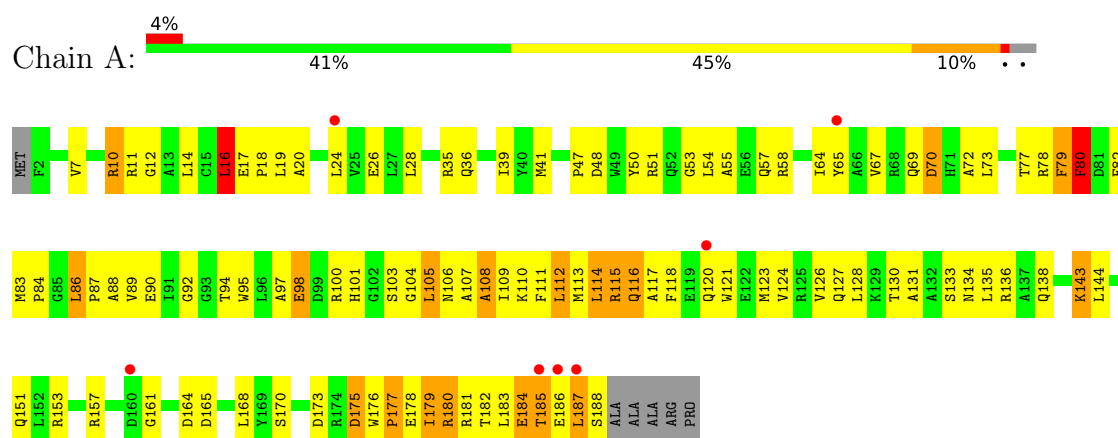
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

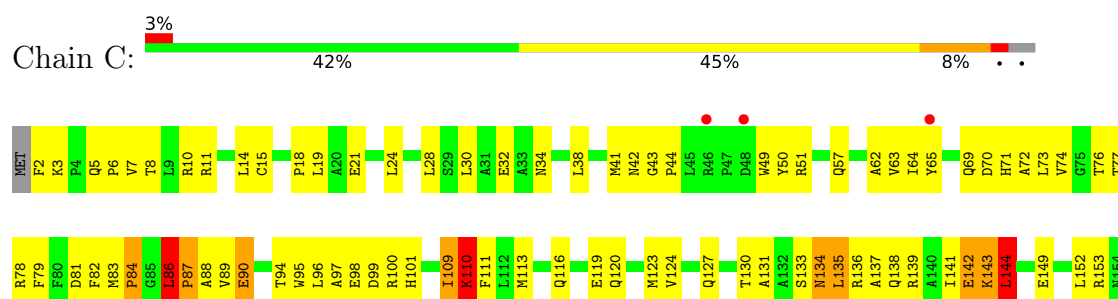
- Molecule 1: GCN5 family acetyltransferase

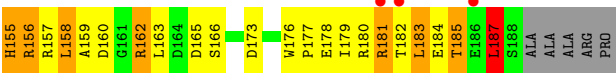


- Molecule 1: GCN5 family acetyltransferase

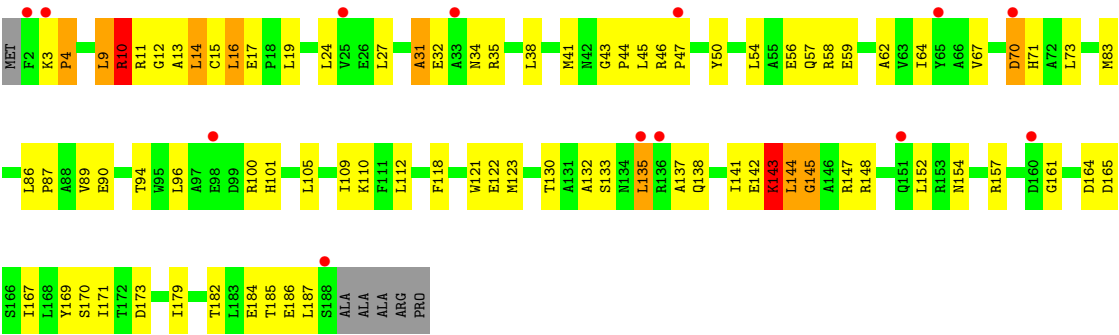


- Molecule 1: GCN5 family acetyltransferase





● Molecule 1: GCN5 family acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.89Å 99.01Å 98.82Å 90.00° 101.87° 90.00°	Depositor
Resolution (Å)	42.95 – 3.04 42.95 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.0 (42.95-3.04) 92.6 (42.95-3.04)	Depositor EDS
R_{merge}	0.47	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.225 , 0.302 0.226 , 0.300	Depositor DCC
R_{free} test set	1593 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6245	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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

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	1.43	27/1532 (1.8%)	1.10	10/2070 (0.5%)
1	B	1.24	21/1532 (1.4%)	1.22	19/2070 (0.9%)
1	C	1.26	24/1532 (1.6%)	1.09	13/2070 (0.6%)
1	D	0.85	12/1532 (0.8%)	0.86	1/2070 (0.0%)
All	All	1.21	84/6128 (1.4%)	1.07	43/8280 (0.5%)

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 (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	VAL	C-O	-9.07	1.13	1.24
1	A	72	ALA	CA-C	-8.69	1.41	1.52
1	A	20	ALA	C-O	-8.63	1.12	1.23
1	C	89	VAL	C-O	-8.00	1.14	1.24
1	B	21	GLU	CA-C	-7.97	1.42	1.52
1	A	112	LEU	CA-C	-7.89	1.42	1.52
1	B	74	VAL	C-O	-7.49	1.15	1.24
1	C	109	ILE	C-O	-7.40	1.15	1.24
1	D	17	GLU	C-O	-7.32	1.14	1.23
1	A	80	PHE	C-O	-7.14	1.17	1.24
1	C	83	MET	C-O	-7.07	1.16	1.24
1	B	21	GLU	C-O	-6.99	1.16	1.24
1	C	90	GLU	C-O	-6.96	1.16	1.23
1	A	70	ASP	CA-C	-6.94	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	ARG	CA-C	-6.91	1.42	1.52
1	A	112	LEU	C-O	-6.89	1.16	1.24
1	A	107	ALA	CA-C	-6.85	1.43	1.52
1	C	185	THR	CA-C	-6.67	1.43	1.52
1	C	162	ARG	CA-C	-6.67	1.44	1.53
1	B	68	ARG	C-O	-6.65	1.15	1.23
1	A	79	PHE	C-O	-6.57	1.15	1.24
1	A	115	ARG	C-O	-6.51	1.15	1.24
1	A	179	ILE	C-O	-6.46	1.15	1.24
1	B	22	ALA	CA-C	-6.42	1.43	1.52
1	A	114	LEU	C-O	-6.33	1.16	1.24
1	D	145	GLY	C-O	-6.30	1.15	1.23
1	D	9	LEU	C-O	-6.30	1.16	1.23
1	D	144	LEU	CA-C	-6.27	1.45	1.52
1	C	88	ALA	C-O	-6.26	1.16	1.23
1	A	106	ASN	CA-C	-6.16	1.45	1.52
1	A	113	MET	C-O	-6.13	1.16	1.24
1	C	111	PHE	C-O	-6.13	1.16	1.24
1	A	108	ALA	C-O	-6.12	1.16	1.24
1	C	187	LEU	C-O	-6.01	1.16	1.23
1	C	183	LEU	C-O	-5.98	1.17	1.24
1	B	74	VAL	CA-C	-5.97	1.45	1.52
1	D	14	LEU	C-O	-5.95	1.16	1.24
1	A	17	GLU	CA-C	-5.95	1.46	1.52
1	B	17	GLU	C-O	-5.93	1.18	1.24
1	D	13	ALA	CA-C	-5.91	1.44	1.52
1	B	69	GLN	C-O	-5.86	1.16	1.23
1	C	181	ARG	C-O	-5.84	1.16	1.24
1	A	16	LEU	C-O	-5.82	1.16	1.24
1	B	18	PRO	C-O	-5.80	1.17	1.23
1	A	107	ALA	C-O	-5.77	1.17	1.24
1	C	110	LYS	C-O	-5.70	1.16	1.24
1	A	180	ARG	CA-C	-5.64	1.45	1.52
1	A	72	ALA	C-O	-5.64	1.17	1.23
1	D	142	GLU	CA-C	-5.63	1.45	1.52
1	C	144	LEU	CA-C	-5.60	1.45	1.52
1	B	24	LEU	CA-C	-5.59	1.44	1.52
1	C	81	ASP	CA-C	-5.58	1.47	1.53
1	C	155	HIS	C-O	-5.56	1.16	1.23
1	D	16	LEU	C-O	-5.55	1.17	1.23
1	A	105	LEU	C-O	-5.54	1.17	1.24
1	D	12	GLY	C-O	-5.54	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	74	VAL	N-CA	-5.52	1.39	1.46
1	A	116	GLN	C-O	-5.52	1.17	1.24
1	C	142	GLU	C-O	-5.51	1.17	1.24
1	A	180	ARG	C-O	-5.50	1.17	1.24
1	C	163	LEU	C-O	-5.44	1.17	1.24
1	C	82	PHE	C-O	-5.39	1.17	1.24
1	B	23	ASP	C-O	-5.38	1.17	1.24
1	B	73	LEU	C-O	-5.38	1.17	1.23
1	B	20	ALA	CA-C	-5.38	1.45	1.53
1	B	73	LEU	CA-C	-5.33	1.45	1.52
1	A	20	ALA	CA-C	-5.32	1.46	1.52
1	B	42	ASN	CA-C	-5.32	1.46	1.52
1	A	17	GLU	C-O	-5.32	1.18	1.24
1	D	142	GLU	C-O	-5.29	1.18	1.24
1	B	86	LEU	C-O	-5.28	1.17	1.24
1	D	10	ARG	C-O	-5.26	1.17	1.23
1	A	10	ARG	C-O	-5.25	1.17	1.23
1	B	87	PRO	C-O	-5.22	1.12	1.23
1	A	175	ASP	C-O	-5.21	1.17	1.24
1	C	88	ALA	CA-C	-5.20	1.46	1.52
1	B	19	LEU	C-O	-5.19	1.18	1.24
1	C	158	LEU	CA-C	-5.14	1.46	1.53
1	A	116	GLN	CA-C	-5.08	1.45	1.52
1	C	185	THR	C-O	-5.05	1.17	1.24
1	C	183	LEU	N-CA	-5.04	1.40	1.46
1	B	84	PRO	C-O	-5.03	1.17	1.24
1	C	144	LEU	C-O	-5.03	1.17	1.24
1	D	143	LYS	C-O	-5.02	1.17	1.24

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	ASP	N-CA-C	-12.73	97.78	113.18
1	C	187	LEU	N-CA-C	-11.60	95.33	112.04
1	B	71	HIS	N-CA-C	-10.20	89.08	110.80
1	A	184	GLU	N-CA-C	-10.19	101.17	114.31
1	B	73	LEU	N-CA-C	-9.18	96.89	110.48
1	C	111	PHE	N-CA-C	-9.09	100.51	111.69
1	B	143	LYS	N-CA-C	-8.57	101.43	112.23
1	C	84	PRO	N-CA-C	8.09	125.80	113.75
1	B	85	GLY	N-CA-C	-7.91	102.92	112.49
1	A	185	THR	N-CA-C	-7.76	101.93	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	GLN	CA-C-N	7.72	133.62	122.35
1	B	69	GLN	C-N-CA	7.72	133.62	122.35
1	A	104	GLY	N-CA-C	7.38	125.55	115.30
1	B	86	LEU	C-N-CD	7.25	136.54	120.60
1	C	86	LEU	C-N-CD	7.14	136.31	120.60
1	B	68	ARG	N-CA-C	7.01	119.82	109.24
1	A	180	ARG	N-CA-C	-6.80	103.56	110.97
1	B	84	PRO	N-CA-C	6.76	122.34	114.03
1	C	110	LYS	N-CA-C	6.69	121.44	113.28
1	B	100	ARG	NE-CZ-NH2	6.62	125.16	119.20
1	A	116	GLN	N-CA-C	-6.40	103.56	112.45
1	C	185	THR	CB-CA-C	-6.28	98.48	109.02
1	B	43	GLY	N-CA-C	-6.17	99.76	112.34
1	B	20	ALA	N-CA-C	-6.14	101.69	110.59
1	B	74	VAL	CB-CA-C	6.06	121.22	111.29
1	B	87	PRO	CA-N-CD	-6.03	103.06	111.50
1	C	89	VAL	CB-CA-C	-5.98	101.49	111.29
1	C	157	ARG	N-CA-C	-5.92	99.24	108.90
1	A	80	PHE	N-CA-C	5.79	115.89	108.24
1	B	72	ALA	N-CA-C	-5.70	95.03	111.00
1	B	86	LEU	N-CA-C	5.70	122.41	109.81
1	C	87	PRO	CA-N-CD	-5.67	103.56	111.50
1	A	79	PHE	CB-CA-C	-5.67	98.54	109.37
1	D	10	ARG	N-CA-C	5.67	117.88	108.13
1	B	21	GLU	CB-CA-C	-5.37	101.88	110.79
1	A	78	ARG	N-CA-C	5.35	117.54	109.41
1	C	155	HIS	N-CA-CB	-5.33	103.50	110.59
1	C	158	LEU	N-CA-C	-5.28	103.07	110.35
1	A	20	ALA	N-CA-C	-5.23	101.46	109.41
1	A	185	THR	CB-CA-C	-5.23	102.01	110.79
1	C	84	PRO	CA-N-CD	-5.21	104.71	112.00
1	B	68	ARG	N-CA-CB	-5.08	102.85	111.69
1	C	144	LEU	N-CA-C	-5.04	107.14	113.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	135	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	1504	0	1509	116	1
1	B	1504	0	1509	121	1
1	C	1504	0	1509	113	0
1	D	1504	0	1509	80	0
2	A	48	0	32	7	0
2	B	48	0	32	5	0
2	C	48	0	32	11	0
2	D	48	0	32	11	0
3	A	13	0	0	0	0
3	B	6	0	0	0	0
3	C	11	0	0	0	0
3	D	7	0	0	0	0
All	All	6245	0	6164	423	1

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 34.

All (423) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:LEU:HD21	1:B:50:TYR:CB	1.16	1.59
1:B:24:LEU:CD2	1:B:50:TYR:HB2	1.35	1.51
1:A:175:ASP:O	1:A:179:ILE:HD13	1.25	1.28
1:B:24:LEU:CD2	1:B:50:TYR:CB	2.02	1.22
2:D:201:COA:O4B	2:D:201:COA:C1B	1.63	1.19
2:B:201:COA:O4B	2:B:201:COA:C1B	1.63	1.18
1:B:24:LEU:CD2	1:B:50:TYR:CG	2.28	1.17
1:A:175:ASP:O	1:A:179:ILE:CD1	1.97	1.12
1:B:26:GLU:OE1	1:B:71:HIS:HE1	1.34	1.11
1:A:14:LEU:HD13	1:A:105:LEU:HD11	1.26	1.07
1:B:97:ALA:HB3	1:B:100:ARG:NH2	1.69	1.05
1:A:182:THR:O	1:A:185:THR:OG1	1.75	1.05
1:A:14:LEU:CD1	1:A:105:LEU:HD11	1.88	1.03
1:C:24:LEU:HD12	1:C:50:TYR:CB	1.90	1.02
1:A:116:GLN:OE1	1:A:120:GLN:CD	2.03	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:MET:O	1:C:159:ALA:HB2	1.61	0.99
1:B:24:LEU:HD21	1:B:50:TYR:CG	1.93	0.99
1:B:26:GLU:OE1	1:B:71:HIS:CE1	2.16	0.98
1:A:116:GLN:OE1	1:A:120:GLN:OE1	1.82	0.98
1:B:24:LEU:HD21	1:B:50:TYR:HB3	1.46	0.97
1:B:24:LEU:CD2	1:B:50:TYR:CD1	2.51	0.94
1:D:35:ARG:HE	1:D:45:LEU:HD13	1.31	0.93
1:B:68:ARG:HG3	1:B:73:LEU:HD23	1.52	0.92
1:A:14:LEU:HD13	1:A:105:LEU:CD1	1.99	0.92
1:B:24:LEU:HD23	1:B:50:TYR:CG	2.02	0.91
1:B:89:VAL:HG22	1:B:123:MET:HE1	1.51	0.90
1:A:185:THR:HG1	1:A:186:GLU:H	1.16	0.90
1:B:138:GLN:O	1:B:142:GLU:HG3	1.72	0.90
1:B:42:ASN:O	1:B:42:ASN:ND2	2.07	0.88
1:A:116:GLN:OE1	1:A:120:GLN:NE2	2.07	0.88
1:C:109:ILE:HG22	1:C:113:MET:HE2	1.55	0.88
1:C:182:THR:O	1:C:185:THR:OG1	1.92	0.87
1:B:97:ALA:HB3	1:B:100:ARG:HH21	1.35	0.86
1:C:24:LEU:CD1	1:C:50:TYR:HB3	2.04	0.86
1:B:24:LEU:HD23	1:B:50:TYR:CD1	2.12	0.84
1:C:139:ARG:NH1	1:C:143:LYS:HG2	1.91	0.84
1:C:110:LYS:NZ	1:C:110:LYS:HB3	1.93	0.84
1:A:186:GLU:OE1	1:A:187:LEU:HD23	1.78	0.83
1:C:24:LEU:HD12	1:C:50:TYR:HB2	1.59	0.83
1:D:132:ALA:HA	1:D:167:ILE:HD11	1.58	0.82
1:B:19:LEU:HD21	1:B:50:TYR:HB3	1.62	0.81
1:B:24:LEU:HD22	1:B:50:TYR:HB2	1.56	0.81
1:D:57:GLN:NE2	1:D:57:GLN:C	2.39	0.81
1:C:86:LEU:HB2	1:C:87:PRO:HA	1.62	0.80
1:B:69:GLN:C	1:B:71:HIS:O	2.25	0.80
1:B:97:ALA:CB	1:B:100:ARG:NH2	2.44	0.80
1:C:24:LEU:HD12	1:C:50:TYR:HB3	1.60	0.80
1:C:90:GLU:HG3	1:C:127:GLN:HG3	1.63	0.80
1:A:14:LEU:HD22	1:A:105:LEU:HD12	1.63	0.78
1:D:10:ARG:N	1:D:10:ARG:HD3	1.99	0.76
1:C:181:ARG:O	1:C:185:THR:HG23	1.84	0.76
1:D:9:LEU:HA	1:D:10:ARG:HH21	1.51	0.76
1:A:135:LEU:HD22	1:C:185:THR:HG21	1.66	0.76
1:A:97:ALA:HB3	1:A:100:ARG:HH11	1.51	0.75
2:A:201:COA:N6A	1:C:185:THR:HG22	2.02	0.75
1:B:43:GLY:O	1:B:49:TRP:CE3	2.41	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:CD2	1:C:185:THR:HG21	2.17	0.74
1:B:70:ASP:O	1:B:71:HIS:HB2	1.87	0.73
1:C:119:GLU:OE1	1:C:176:TRP:NE1	2.18	0.73
1:B:181:ARG:HH22	1:D:135:LEU:HB3	1.54	0.72
1:C:95:TRP:HA	2:C:201:COA:CDP	2.19	0.72
1:D:137:ALA:O	1:D:141:ILE:HG13	1.90	0.71
1:A:28:LEU:HD22	1:A:47:PRO:HG3	1.73	0.71
1:A:14:LEU:HD22	1:A:105:LEU:CD1	2.19	0.71
1:B:43:GLY:H	1:B:44:PRO:HD3	1.56	0.70
1:A:176:TRP:HB3	1:A:177:PRO:HD3	1.73	0.70
1:D:24:LEU:HD21	1:D:47:PRO:HA	1.74	0.70
1:D:141:ILE:HD11	2:D:201:COA:H21	1.73	0.69
1:C:136:ARG:HH21	2:C:201:COA:H52A	1.58	0.69
1:C:138:GLN:O	1:C:142:GLU:HG3	1.93	0.69
1:B:92:GLY:HA2	2:B:201:COA:H32	1.74	0.69
1:B:97:ALA:CB	1:B:100:ARG:HH22	2.05	0.69
1:D:143:LYS:HE2	2:D:201:COA:O2A	1.92	0.68
1:A:185:THR:HG1	1:A:186:GLU:N	1.88	0.68
1:A:16:LEU:HD21	1:A:109:ILE:HG23	1.75	0.68
1:D:101:HIS:NE2	2:D:201:COA:OAP	2.27	0.68
1:D:171:ILE:HD12	1:D:179:ILE:HG13	1.76	0.68
1:C:11:ARG:HH21	1:C:187:LEU:CD2	2.08	0.67
1:D:157:ARG:NH1	1:D:161:GLY:O	2.24	0.67
1:B:43:GLY:H	1:B:44:PRO:CD	2.07	0.66
1:A:82:PHE:CD1	1:A:89:VAL:HG23	2.31	0.66
1:C:96:LEU:HD21	1:C:109:ILE:HD11	1.77	0.66
1:B:59:GLU:N	1:B:59:GLU:OE1	2.28	0.66
1:A:151:GLN:NE2	1:A:165:ASP:OD2	2.28	0.65
1:C:86:LEU:CB	1:C:87:PRO:HA	2.21	0.65
1:D:148:ARG:HG3	1:D:169:TYR:CE2	2.31	0.65
1:B:68:ARG:HG3	1:B:73:LEU:CD2	2.24	0.65
1:D:14:LEU:HD13	1:D:105:LEU:HD21	1.79	0.65
1:B:38:LEU:CD2	1:B:95:TRP:HB2	2.27	0.65
1:B:24:LEU:HD21	1:B:50:TYR:HB2	0.65	0.64
1:B:183:LEU:O	1:B:187:LEU:HG	1.97	0.64
1:A:82:PHE:CE1	1:A:89:VAL:HG23	2.32	0.64
1:C:87:PRO:HD2	1:C:123:MET:HA	1.79	0.64
1:C:11:ARG:HE	1:C:187:LEU:HD21	1.62	0.64
1:A:178:GLU:OE1	1:A:181:ARG:HD2	1.97	0.64
1:D:43:GLY:O	1:D:45:LEU:N	2.31	0.63
1:B:174:ARG:NH2	1:D:154:ASN:OD1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:THR:HB	2:D:201:COA:H31	1.81	0.63
1:B:19:LEU:HD13	1:B:64:ILE:HG12	1.81	0.62
1:A:180:ARG:O	1:A:184:GLU:HG3	1.99	0.62
1:C:109:ILE:CG2	1:C:113:MET:HE2	2.28	0.62
1:B:14:LEU:HD11	1:B:67:VAL:HG13	1.82	0.62
1:B:89:VAL:HG13	1:B:123:MET:SD	2.40	0.62
1:A:133:SER:OG	1:A:164:ASP:OD2	2.14	0.62
1:D:19:LEU:HG	1:D:54:LEU:HD21	1.81	0.62
1:B:183:LEU:C	1:B:185:THR:H	2.06	0.61
1:C:152:LEU:HD12	1:C:155:HIS:CE1	2.34	0.61
1:B:28:LEU:HD11	1:B:45:LEU:O	2.00	0.61
1:C:139:ARG:NH1	1:C:143:LYS:CG	2.64	0.61
1:A:175:ASP:C	1:A:179:ILE:HD13	2.17	0.61
1:D:130:THR:O	1:D:167:ILE:HD12	2.00	0.61
1:C:110:LYS:HD2	1:C:144:LEU:HD11	1.81	0.61
1:B:100:ARG:O	1:B:103:SER:OG	2.12	0.61
1:A:24:LEU:CD1	1:A:51:ARG:HG3	2.29	0.61
1:C:41:MET:O	1:C:159:ALA:CB	2.46	0.61
1:C:110:LYS:HB3	1:C:110:LYS:HZ2	1.61	0.60
1:B:181:ARG:HH12	1:D:135:LEU:HB2	1.67	0.60
2:B:201:COA:H131	2:B:201:COA:H72	1.84	0.60
1:C:84:PRO:C	1:C:86:LEU:H	2.09	0.60
1:D:46:ARG:HD2	1:D:47:PRO:HD2	1.84	0.60
1:D:143:LYS:CE	2:D:201:COA:O2A	2.49	0.60
1:D:57:GLN:C	1:D:57:GLN:HE21	2.07	0.60
1:B:43:GLY:O	1:B:49:TRP:CD2	2.55	0.59
1:B:26:GLU:CD	1:B:71:HIS:CE1	2.81	0.59
1:D:135:LEU:HA	1:D:138:GLN:HB2	1.85	0.59
1:B:157:ARG:NH1	1:A:86:LEU:O	2.28	0.59
1:A:182:THR:C	1:A:184:GLU:H	2.11	0.59
1:C:136:ARG:NH2	2:C:201:COA:H52A	2.17	0.58
1:C:64:ILE:HD12	1:C:65:TYR:H	1.68	0.58
1:C:183:LEU:C	1:C:185:THR:H	2.10	0.58
2:B:201:COA:O9A	2:B:201:COA:O2B	2.18	0.58
1:C:24:LEU:HD11	1:C:50:TYR:HB3	1.85	0.58
1:C:110:LYS:HB3	1:C:110:LYS:HZ3	1.66	0.58
1:B:86:LEU:HB2	1:B:87:PRO:HA	1.85	0.58
1:B:100:ARG:HH21	1:B:100:ARG:HG2	1.69	0.58
1:D:58:ARG:HB3	1:D:59:GLU:OE1	2.03	0.58
1:B:138:GLN:O	1:B:142:GLU:CG	2.49	0.58
1:A:130:THR:OG1	1:A:131:ALA:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:THR:O	1:B:185:THR:HB	2.04	0.57
1:A:157:ARG:NH1	1:A:161:GLY:O	2.35	0.57
1:B:26:GLU:OE2	1:B:71:HIS:ND1	2.37	0.57
1:B:28:LEU:HD13	1:B:47:PRO:HB3	1.87	0.57
1:A:179:ILE:N	1:A:179:ILE:HD12	2.19	0.57
1:A:109:ILE:O	1:A:109:ILE:HG22	2.04	0.57
1:B:28:LEU:HD21	1:B:47:PRO:HD3	1.86	0.57
1:C:38:LEU:HD13	1:C:44:PRO:HB2	1.87	0.57
1:A:108:ALA:O	1:A:112:LEU:HG	2.04	0.57
1:C:110:LYS:CD	1:C:144:LEU:HD11	2.35	0.56
1:A:131:ALA:O	1:A:138:GLN:NE2	2.37	0.56
1:C:136:ARG:HE	2:C:201:COA:H51A	1.71	0.56
1:B:135:LEU:HD23	1:B:138:GLN:OE1	2.06	0.56
1:A:19:LEU:HB3	1:A:54:LEU:HD21	1.87	0.56
1:A:183:LEU:O	1:A:187:LEU:HD21	2.05	0.56
1:A:183:LEU:O	1:A:187:LEU:HG	2.06	0.56
1:A:24:LEU:HD11	1:A:54:LEU:HD12	1.88	0.56
1:A:178:GLU:O	1:A:182:THR:HG23	2.06	0.56
2:C:201:COA:H4B	2:C:201:COA:O2A	2.05	0.55
1:D:19:LEU:HB3	1:D:64:ILE:HG23	1.88	0.55
1:D:57:GLN:NE2	1:D:57:GLN:O	2.39	0.55
1:B:24:LEU:HD22	1:B:50:TYR:CD1	2.38	0.55
1:B:124:VAL:HA	1:B:173:ASP:HB3	1.88	0.55
1:B:28:LEU:CD2	1:B:47:PRO:HD3	2.35	0.55
1:C:2:PHE:HD1	1:C:3:LYS:N	2.05	0.55
1:D:70:ASP:OD2	1:D:71:HIS:ND1	2.40	0.55
1:C:64:ILE:HD13	1:C:78:ARG:NE	2.21	0.55
1:D:145:GLY:HA3	1:D:179:ILE:HD12	1.88	0.55
1:B:181:ARG:NH2	1:D:135:LEU:HB3	2.20	0.55
1:B:28:LEU:HD21	1:B:45:LEU:O	2.06	0.55
1:A:89:VAL:HB	1:A:123:MET:SD	2.47	0.54
1:A:117:ALA:O	1:A:123:MET:HB2	2.06	0.54
1:A:19:LEU:CD2	1:A:64:ILE:HG12	2.38	0.54
1:A:10:ARG:NH1	1:A:12:GLY:O	2.40	0.54
1:A:24:LEU:HD21	1:A:54:LEU:HD11	1.90	0.54
1:A:134:ASN:HD21	2:A:201:COA:H71	1.72	0.54
1:C:11:ARG:HH21	1:C:187:LEU:HD23	1.73	0.54
1:C:30:LEU:O	1:C:34:ASN:ND2	2.38	0.54
1:B:19:LEU:HD13	1:B:64:ILE:CG1	2.38	0.54
1:B:153:ARG:NH1	1:A:170:SER:O	2.41	0.54
1:A:14:LEU:CD2	1:A:105:LEU:CD1	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LEU:O	1:A:187:LEU:CG	2.56	0.54
1:C:86:LEU:CB	1:C:87:PRO:CA	2.85	0.54
1:C:110:LYS:HD3	1:C:144:LEU:HD21	1.89	0.54
1:B:174:ARG:HD3	1:D:165:ASP:OD1	2.08	0.53
1:A:14:LEU:CD2	1:A:105:LEU:HD12	2.36	0.53
1:A:182:THR:C	1:A:185:THR:OG1	2.49	0.53
1:A:131:ALA:HB3	1:A:134:ASN:HB2	1.89	0.53
2:D:201:COA:H143	2:D:201:COA:O4A	2.08	0.53
1:B:11:ARG:HB3	1:B:112:LEU:HD11	1.90	0.53
1:C:5:GLN:HG2	1:C:6:PRO:O	2.09	0.53
1:C:139:ARG:HH11	1:C:143:LYS:HG2	1.73	0.53
1:D:184:GLU:HA	1:D:187:LEU:HD12	1.90	0.53
1:B:32:GLU:HB2	1:B:45:LEU:HD23	1.91	0.53
1:C:63:VAL:HG23	1:C:79:PHE:HB2	1.91	0.53
1:C:99:ASP:HB2	1:C:100:ARG:NH2	2.24	0.53
1:C:43:GLY:HA3	1:C:49:TRP:CD1	2.44	0.53
1:D:118:PHE:O	1:D:122:GLU:HA	2.09	0.53
1:C:69:GLN:O	1:C:72:ALA:N	2.31	0.53
1:A:185:THR:OG1	1:A:186:GLU:N	2.33	0.53
1:C:76:THR:O	1:C:94:THR:HA	2.09	0.53
1:A:136:ARG:HG2	2:A:201:COA:H122	1.91	0.52
1:A:182:THR:C	1:A:185:THR:HG1	2.00	0.52
1:D:9:LEU:HB2	1:D:16:LEU:HD12	1.91	0.52
1:B:86:LEU:N	1:B:86:LEU:CD1	2.73	0.52
1:A:65:TYR:HB2	1:A:77:THR:O	2.10	0.52
1:D:50:TYR:O	1:D:54:LEU:HG	2.09	0.52
1:D:11:ARG:HB2	1:D:112:LEU:HD11	1.90	0.52
1:B:49:TRP:HZ3	1:B:95:TRP:HE1	1.57	0.51
1:D:96:LEU:HD21	1:D:109:ILE:HD11	1.91	0.51
1:A:176:TRP:HB3	1:A:177:PRO:CD	2.40	0.51
1:C:177:PRO:O	1:C:181:ARG:HB2	2.10	0.51
1:D:24:LEU:HD11	1:D:47:PRO:HB3	1.92	0.51
1:B:44:PRO:HD2	1:B:45:LEU:H	1.74	0.51
1:A:114:LEU:CD2	1:A:126:VAL:HG11	2.40	0.51
1:B:87:PRO:HD2	1:B:123:MET:HA	1.93	0.51
1:B:110:LYS:HG3	1:B:144:LEU:HD11	1.92	0.51
1:A:11:ARG:NH2	1:A:187:LEU:HB3	2.26	0.51
1:D:147:ARG:NE	1:D:148:ARG:O	2.37	0.51
1:D:32:GLU:OE1	1:D:35:ARG:NH1	2.44	0.51
1:C:149:GLU:OE1	1:D:152:LEU:HD22	2.11	0.50
1:D:182:THR:O	1:D:185:THR:OG1	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ARG:CZ	1:D:135:LEU:H	2.23	0.50
1:C:7:VAL:O	1:C:65:TYR:OH	2.22	0.50
1:C:24:LEU:CD1	1:C:50:TYR:CB	2.65	0.50
1:D:24:LEU:HD23	1:D:50:TYR:HB2	1.92	0.50
1:D:182:THR:O	1:D:186:GLU:HG2	2.11	0.50
1:C:179:ILE:O	1:C:182:THR:HG22	2.11	0.50
1:D:89:VAL:HB	1:D:123:MET:SD	2.52	0.50
1:B:86:LEU:HD13	1:B:86:LEU:H	1.76	0.49
1:B:28:LEU:HD11	1:B:45:LEU:C	2.38	0.49
1:A:79:PHE:CE1	1:A:121:TRP:HZ3	2.30	0.49
1:C:178:GLU:O	1:C:179:ILE:HD13	2.11	0.49
1:B:16:LEU:HD21	1:B:67:VAL:HG22	1.93	0.49
1:B:154:ASN:HD22	1:A:124:VAL:HG22	1.77	0.49
1:A:14:LEU:HD11	1:A:105:LEU:HD11	1.89	0.49
2:A:201:COA:H61A	1:C:185:THR:HG22	1.76	0.49
1:D:11:ARG:NH1	1:D:187:LEU:HD22	2.28	0.49
1:B:69:GLN:O	1:B:71:HIS:O	2.31	0.49
1:A:24:LEU:HD22	1:A:50:TYR:HB3	1.94	0.49
1:B:158:LEU:C	1:B:160:ASP:H	2.21	0.49
1:A:14:LEU:CD1	1:A:105:LEU:CD1	2.73	0.49
1:B:111:PHE:HB2	1:B:183:LEU:HD13	1.93	0.49
1:C:21:GLU:HG3	1:C:51:ARG:HH22	1.78	0.48
1:C:94:THR:O	2:C:201:COA:H72	2.13	0.48
1:D:121:TRP:C	1:D:122:GLU:HG2	2.38	0.48
1:B:41:MET:O	1:B:41:MET:HG3	2.13	0.48
1:C:110:LYS:HE3	2:C:201:COA:S1P	2.53	0.48
1:B:16:LEU:CD2	1:B:67:VAL:HG22	2.42	0.48
1:C:24:LEU:N	1:C:24:LEU:HD22	2.28	0.48
1:C:156:ARG:NE	1:C:166:SER:OG	2.46	0.48
1:D:94:THR:O	2:D:201:COA:H62	2.14	0.48
1:A:26:GLU:HB3	1:A:73:LEU:HD13	1.95	0.48
1:A:54:LEU:O	1:A:57:GLN:HB3	2.13	0.48
1:B:26:GLU:O	1:B:26:GLU:HG2	2.13	0.48
1:C:158:LEU:HD12	1:C:162:ARG:NE	2.29	0.48
1:C:176:TRP:NE1	1:C:180:ARG:HH21	2.11	0.48
1:D:83:MET:O	1:D:87:PRO:HA	2.14	0.48
1:C:11:ARG:NH2	1:C:187:LEU:CD2	2.75	0.47
1:B:100:ARG:HD3	1:B:100:ARG:N	2.27	0.47
1:B:181:ARG:NH1	1:D:135:LEU:HB2	2.27	0.47
1:A:182:THR:C	1:A:184:GLU:N	2.72	0.47
1:D:10:ARG:HD3	1:D:10:ARG:H	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLU:OE1	1:B:180:ARG:NH2	2.46	0.47
1:B:135:LEU:HA	1:B:138:GLN:OE1	2.14	0.47
1:B:151:GLN:HA	1:B:166:SER:O	2.15	0.47
1:B:183:LEU:O	1:B:185:THR:N	2.47	0.47
1:B:186:GLU:O	1:B:186:GLU:HG2	2.14	0.47
1:A:80:PHE:CD1	1:A:90:GLU:HB3	2.49	0.47
1:A:118:PHE:HE2	1:A:173:ASP:HA	1.79	0.47
1:D:27:LEU:HG	1:D:73:LEU:HD21	1.96	0.47
1:A:16:LEU:HD23	1:A:67:VAL:HG22	1.96	0.47
1:B:19:LEU:HD13	1:B:64:ILE:CD1	2.44	0.47
1:A:19:LEU:HD23	1:A:64:ILE:CD1	2.44	0.47
1:A:124:VAL:HG23	1:A:173:ASP:OD2	2.14	0.47
1:C:124:VAL:HG23	1:D:154:ASN:HB3	1.97	0.47
1:B:176:TRP:CZ2	1:B:180:ARG:HB2	2.50	0.47
1:B:158:LEU:HD12	1:B:162:ARG:HH11	1.79	0.47
1:A:182:THR:HA	1:A:185:THR:CG2	2.44	0.47
1:A:135:LEU:HD23	1:C:185:THR:HG21	1.94	0.47
1:C:7:VAL:HG23	1:C:65:TYR:OH	2.14	0.47
1:C:95:TRP:HA	2:C:201:COA:H132	1.95	0.47
1:A:118:PHE:CE2	1:A:173:ASP:HA	2.50	0.46
1:B:183:LEU:C	1:B:185:THR:N	2.68	0.46
1:C:11:ARG:NE	1:C:187:LEU:HD21	2.29	0.46
1:C:10:ARG:HG2	1:C:11:ARG:N	2.28	0.46
1:B:139:ARG:HA	1:B:142:GLU:HG3	1.97	0.46
2:B:201:COA:H131	2:B:201:COA:C7P	2.45	0.46
1:C:183:LEU:C	1:C:185:THR:N	2.73	0.46
1:D:56:GLU:O	1:D:62:ALA:N	2.48	0.46
1:B:19:LEU:HD13	1:B:64:ILE:HD11	1.98	0.46
1:A:41:MET:HE1	1:A:95:TRP:CD1	2.50	0.46
1:C:98:GLU:C	1:C:100:ARG:H	2.24	0.46
1:A:101:HIS:C	1:A:103:SER:H	2.24	0.46
1:A:183:LEU:O	1:A:187:LEU:CD2	2.63	0.46
1:C:84:PRO:C	1:C:86:LEU:N	2.72	0.46
2:C:201:COA:N8P	2:C:201:COA:H133	2.30	0.46
1:A:110:LYS:HG3	1:A:144:LEU:HD21	1.98	0.46
1:C:134:ASN:O	1:C:136:ARG:N	2.48	0.46
1:C:158:LEU:CD1	1:C:162:ARG:NH1	2.78	0.46
1:A:98:GLU:HA	1:A:101:HIS:NE2	2.30	0.46
1:C:70:ASP:O	1:C:71:HIS:ND1	2.48	0.46
1:A:82:PHE:CE1	1:A:89:VAL:CG2	2.99	0.46
1:B:152:LEU:HD22	1:A:168:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:LEU:HD23	1:C:158:LEU:HA	1.78	0.45
1:A:181:ARG:HD3	1:A:182:THR:CG2	2.47	0.45
1:D:31:ALA:HB1	1:D:45:LEU:HD23	1.98	0.45
1:B:36:GLN:O	1:B:39:ILE:HG23	2.15	0.45
1:C:153:ARG:NH1	1:D:170:SER:O	2.49	0.45
1:B:162:ARG:HE	1:B:162:ARG:HB3	1.53	0.45
1:B:43:GLY:N	1:B:44:PRO:HD3	2.28	0.45
1:A:19:LEU:HG	1:A:54:LEU:HD21	1.99	0.45
1:C:57:GLN:HA	1:C:62:ALA:O	2.15	0.45
1:D:14:LEU:HD11	1:D:67:VAL:CG1	2.47	0.45
1:C:14:LEU:HD12	1:C:15:CYS:H	1.82	0.45
1:B:68:ARG:HG2	1:B:71:HIS:HA	1.97	0.45
1:B:176:TRP:CH2	1:B:180:ARG:HB2	2.52	0.45
1:C:130:THR:OG1	1:C:131:ALA:N	2.49	0.45
1:C:143:LYS:HD2	1:C:143:LYS:HA	1.70	0.44
1:B:71:HIS:HB3	1:B:72:ALA:HA	1.99	0.44
1:A:80:PHE:CE1	1:A:90:GLU:CD	2.95	0.44
1:A:143:LYS:HE2	2:A:201:COA:H4B	1.98	0.44
1:A:36:GLN:O	1:A:39:ILE:HG12	2.18	0.44
1:C:156:ARG:HD2	1:C:165:ASP:O	2.16	0.44
1:B:170:SER:OG	1:A:153:ARG:NH1	2.44	0.44
1:C:28:LEU:O	1:C:32:GLU:N	2.43	0.44
1:C:42:ASN:HA	1:C:159:ALA:HB2	1.98	0.44
1:D:57:GLN:HE21	1:D:58:ARG:N	2.15	0.44
1:C:133:SER:O	1:C:135:LEU:N	2.48	0.44
1:D:100:ARG:HA	1:D:100:ARG:HD3	1.54	0.44
1:A:115:ARG:O	1:A:115:ARG:HG2	2.18	0.44
1:D:41:MET:HB3	1:D:41:MET:HE2	1.82	0.44
1:C:137:ALA:O	1:C:141:ILE:HG13	2.18	0.44
1:D:143:LYS:NZ	1:D:143:LYS:HB2	2.32	0.44
1:D:157:ARG:HB3	1:D:161:GLY:HA2	2.00	0.44
1:B:3:LYS:HE3	1:B:5:GLN:HE22	1.83	0.43
1:B:86:LEU:CB	1:B:87:PRO:CA	2.96	0.43
1:A:175:ASP:O	1:A:179:ILE:HD12	2.06	0.43
2:D:201:COA:H8A	2:D:201:COA:H2B	1.74	0.43
1:A:182:THR:HA	1:A:185:THR:OG1	2.18	0.43
1:A:182:THR:HA	1:A:185:THR:HG23	1.99	0.43
1:A:182:THR:OG1	1:A:183:LEU:N	2.49	0.43
1:C:38:LEU:HB3	1:C:44:PRO:HG3	1.99	0.43
1:C:65:TYR:HB2	1:C:77:THR:O	2.19	0.43
1:B:86:LEU:HB2	1:B:87:PRO:CA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:PRO:C	1:B:49:TRP:N	2.72	0.43
1:D:41:MET:SD	2:D:201:COA:H61	2.59	0.43
1:D:46:ARG:HH11	1:D:47:PRO:HD2	1.83	0.43
1:B:16:LEU:HD11	1:B:109:ILE:HG23	1.99	0.43
1:A:83:MET:HE3	1:A:86:LEU:HD12	1.99	0.43
2:C:201:COA:O2A	2:C:201:COA:C4B	2.67	0.43
1:A:88:ALA:HA	1:A:123:MET:HG2	2.01	0.43
1:A:128:LEU:N	1:A:128:LEU:HD12	2.34	0.43
1:C:63:VAL:CG2	1:C:79:PHE:HB2	2.48	0.43
1:B:11:ARG:NH2	1:B:187:LEU:HB3	2.33	0.43
1:C:116:GLN:HA	1:C:120:GLN:HB2	1.99	0.43
1:C:183:LEU:O	1:C:185:THR:N	2.52	0.43
1:D:10:ARG:O	1:D:10:ARG:HG2	2.19	0.43
1:D:34:ASN:O	1:D:38:LEU:HG	2.18	0.43
1:A:53:GLY:HA3	1:A:64:ILE:CD1	2.49	0.43
1:C:152:LEU:HD12	1:C:155:HIS:NE2	2.33	0.43
1:C:19:LEU:HB3	1:C:64:ILE:HG23	2.00	0.43
1:D:110:LYS:HA	1:D:110:LYS:HD3	1.78	0.43
1:C:124:VAL:HA	1:C:173:ASP:HB3	2.00	0.43
1:C:99:ASP:C	1:C:100:ARG:HD3	2.43	0.42
1:D:9:LEU:C	1:D:10:ARG:HD3	2.43	0.42
1:B:144:LEU:HD23	1:B:144:LEU:HA	1.77	0.42
1:B:154:ASN:ND2	1:A:124:VAL:HG22	2.34	0.42
1:A:55:ALA:HA	1:A:58:ARG:NH2	2.35	0.42
1:A:90:GLU:HG3	1:A:127:GLN:O	2.18	0.42
1:C:43:GLY:N	1:C:44:PRO:CD	2.83	0.42
1:A:181:ARG:HD3	1:A:182:THR:HG22	2.01	0.42
1:A:111:PHE:CZ	1:A:184:GLU:OE2	2.72	0.42
1:A:118:PHE:HE1	1:A:126:VAL:HB	1.83	0.42
1:C:185:THR:H	1:C:185:THR:HG1	1.63	0.42
1:D:144:LEU:HD23	1:D:144:LEU:HA	1.84	0.42
1:A:83:MET:O	1:A:87:PRO:HA	2.19	0.42
1:B:90:GLU:HG2	1:B:91:ILE:O	2.19	0.42
1:C:97:ALA:HB3	1:C:100:ARG:NH2	2.34	0.42
1:D:10:ARG:N	1:D:10:ARG:CD	2.71	0.42
1:D:173:ASP:OD1	1:D:173:ASP:N	2.51	0.42
1:B:3:LYS:HE3	1:B:5:GLN:NE2	2.35	0.42
1:A:48:ASP:HA	1:A:51:ARG:HB2	2.00	0.42
1:A:77:THR:HG21	1:A:109:ILE:HG21	2.01	0.42
1:C:3:LYS:HD2	1:C:3:LYS:HA	1.75	0.42
1:D:9:LEU:HA	1:D:10:ARG:NH2	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:201:COA:N3A	2:A:201:COA:H2B	2.34	0.42
1:D:3:LYS:HA	1:D:4:PRO:HD3	1.78	0.42
1:B:153:ARG:H	1:B:153:ARG:HG3	1.57	0.41
1:C:98:GLU:C	1:C:100:ARG:N	2.77	0.41
1:B:73:LEU:HD23	1:B:73:LEU:HA	1.81	0.41
1:A:84:PRO:C	1:A:86:LEU:H	2.28	0.41
1:B:38:LEU:HD21	1:B:95:TRP:CE3	2.55	0.41
1:B:82:PHE:CD1	1:B:89:VAL:HG12	2.54	0.41
1:A:117:ALA:O	1:A:121:TRP:HB2	2.21	0.41
1:D:182:THR:C	1:D:185:THR:HG1	2.21	0.41
1:C:101:HIS:CE1	2:C:201:COA:H143	2.56	0.41
1:C:158:LEU:HD12	1:C:162:ARG:HE	1.84	0.41
1:B:28:LEU:O	1:B:31:ALA:N	2.53	0.41
1:A:92:GLY:C	1:A:94:THR:N	2.78	0.41
2:A:201:COA:O7A	2:A:201:COA:C4B	2.68	0.41
1:B:3:LYS:HE3	1:B:5:GLN:OE1	2.21	0.41
1:A:7:VAL:HG11	1:A:116:GLN:NE2	2.36	0.41
1:A:19:LEU:HD23	1:A:64:ILE:HD11	2.03	0.41
1:C:8:THR:HG22	1:C:18:PRO:HD3	2.03	0.41
1:D:89:VAL:HG22	1:D:90:GLU:N	2.36	0.41
1:D:101:HIS:CE1	2:D:201:COA:OAP	2.73	0.41
1:B:55:ALA:O	1:B:57:GLN:N	2.54	0.41
1:B:76:THR:O	1:B:94:THR:HA	2.21	0.41
1:B:79:PHE:O	1:B:80:PHE:HB3	2.21	0.41
1:B:147:ARG:O	1:B:169:TYR:HA	2.20	0.41
1:C:18:PRO:HA	1:C:64:ILE:O	2.21	0.41
1:C:64:ILE:HD13	1:C:78:ARG:HE	1.83	0.41
1:C:73:LEU:HA	1:C:73:LEU:HD13	1.83	0.41
1:C:176:TRP:CD1	1:C:180:ARG:HH21	2.39	0.41
1:C:141:ILE:O	1:C:144:LEU:HB2	2.21	0.41
1:B:42:ASN:ND2	1:B:42:ASN:C	2.70	0.40
1:A:105:LEU:O	1:A:109:ILE:HG13	2.21	0.40
1:C:135:LEU:HD23	1:C:135:LEU:HA	1.80	0.40
1:A:19:LEU:CB	1:A:54:LEU:HD21	2.50	0.40
1:A:79:PHE:CE1	1:A:121:TRP:CZ3	3.08	0.40
1:D:11:ARG:CZ	1:D:187:LEU:HD22	2.52	0.40
1:D:133:SER:OG	1:D:164:ASP:OD2	2.22	0.40
1:B:87:PRO:HB2	1:B:123:MET:HG2	2.03	0.40
1:A:53:GLY:HA3	1:A:64:ILE:HD13	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ARG:NH2	1:A:188:SER:O[2_545]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	185/193 (96%)	164 (89%)	18 (10%)	3 (2%)	7	30
1	B	185/193 (96%)	160 (86%)	17 (9%)	8 (4%)	2	11
1	C	185/193 (96%)	166 (90%)	14 (8%)	5 (3%)	4	19
1	D	185/193 (96%)	166 (90%)	14 (8%)	5 (3%)	4	19
All	All	740/772 (96%)	656 (89%)	63 (8%)	21 (3%)	4	18

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	44	PRO
1	B	56	GLU
1	C	86	LEU
1	D	4	PRO
1	B	71	HIS
1	C	184	GLU
1	B	4	PRO
1	B	55	ALA
1	A	70	ASP
1	C	134	ASN
1	C	135	LEU
1	D	31	ALA
1	D	44	PRO
1	D	70	ASP
1	B	184	GLU
1	A	86	LEU
1	A	98	GLU

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Mol	Chain	Res	Type
1	B	86	LEU
1	D	86	LEU
1	C	74	VAL
1	B	43	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	154/157 (98%)	146 (95%)	8 (5%)	21	51
1	B	154/157 (98%)	143 (93%)	11 (7%)	13	40
1	C	154/157 (98%)	148 (96%)	6 (4%)	28	59
1	D	154/157 (98%)	151 (98%)	3 (2%)	50	73
All	All	616/628 (98%)	588 (96%)	28 (4%)	24	56

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	17	GLU
1	B	19	LEU
1	B	21	GLU
1	B	42	ASN
1	B	45	LEU
1	B	48	ASP
1	B	71	HIS
1	B	86	LEU
1	B	100	ARG
1	B	142	GLU
1	B	143	LYS
1	A	16	LEU
1	A	18	PRO
1	A	35	ARG
1	A	69	GLN
1	A	80	PHE
1	A	143	LYS

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Mol	Chain	Res	Type
1	A	177	PRO
1	A	187	LEU
1	C	110	LYS
1	C	143	LYS
1	C	144	LEU
1	C	156	ARG
1	C	160	ASP
1	C	187	LEU
1	D	10	ARG
1	D	15	CYS
1	D	143	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	42	ASN
1	B	71	HIS
1	A	134	ASN
1	C	42	ASN
1	D	57	GLN
1	D	138	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	B	201	-	47,50,50	3.24	20 (42%)	69,75,75	2.60	21 (30%)
2	COA	D	201	-	47,50,50	3.33	23 (48%)	69,75,75	2.58	24 (34%)
2	COA	C	201	-	47,50,50	2.16	18 (38%)	69,75,75	2.54	24 (34%)
2	COA	A	201	-	47,50,50	1.94	13 (27%)	69,75,75	2.40	22 (31%)

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	B	201	-	-	24/48/64/64	0/3/3/3
2	COA	D	201	-	-	24/48/64/64	0/3/3/3
2	COA	C	201	-	-	15/48/64/64	0/3/3/3
2	COA	A	201	-	-	28/48/64/64	0/3/3/3

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	COA	O4B-C1B	9.48	1.63	1.42
2	D	201	COA	C9P-N8P	9.37	1.55	1.33
2	B	201	COA	O4B-C1B	9.33	1.63	1.42
2	B	201	COA	C9P-N8P	8.98	1.54	1.33
2	B	201	COA	P1A-O3A	7.31	1.67	1.59
2	B	201	COA	C2B-C1B	-6.63	1.32	1.53
2	D	201	COA	O4B-C4B	-6.40	1.30	1.45
2	D	201	COA	C2B-C1B	-6.40	1.33	1.53
2	B	201	COA	O4B-C4B	-6.39	1.30	1.45
2	D	201	COA	P2A-O3A	6.03	1.66	1.59
2	D	201	COA	P1A-O3A	5.80	1.65	1.59
2	B	201	COA	P2A-O3A	5.45	1.65	1.59
2	D	201	COA	C6P-C5P	4.95	1.61	1.51
2	A	201	COA	C5A-C4A	4.55	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	COA	P2A-O3A	-4.54	1.54	1.59
2	D	201	COA	CCP-CBP	4.42	1.59	1.52
2	D	201	COA	O5P-C5P	-4.40	1.14	1.23
2	B	201	COA	O5P-C5P	-4.37	1.14	1.23
2	C	201	COA	C4A-N9A	-4.36	1.28	1.37
2	A	201	COA	P1A-O3A	-4.27	1.54	1.59
2	C	201	COA	C5A-N7A	-3.98	1.31	1.39
2	C	201	COA	O5P-C5P	-3.96	1.15	1.23
2	C	201	COA	C2A-N3A	-3.91	1.27	1.33
2	A	201	COA	C5A-N7A	-3.90	1.32	1.39
2	D	201	COA	C7P-N8P	3.76	1.54	1.46
2	B	201	COA	C6P-C5P	3.65	1.58	1.51
2	A	201	COA	C4A-N9A	-3.62	1.30	1.37
2	B	201	COA	C5P-N4P	3.58	1.41	1.33
2	B	201	COA	C6A-N6A	3.53	1.43	1.34
2	C	201	COA	P1A-O1A	-3.53	1.38	1.50
2	A	201	COA	CEP-CBP	-3.48	1.46	1.53
2	D	201	COA	C6A-N6A	3.43	1.43	1.34
2	C	201	COA	C3B-C4B	-3.40	1.44	1.52
2	B	201	COA	C7P-N8P	3.22	1.53	1.46
2	C	201	COA	P1A-O2A	-3.04	1.41	1.55
2	C	201	COA	O9P-C9P	-3.01	1.17	1.23
2	D	201	COA	C5P-N4P	2.95	1.40	1.33
2	C	201	COA	P1A-O3A	-2.94	1.56	1.59
2	D	201	COA	O3B-C3B	-2.94	1.34	1.44
2	C	201	COA	P2A-O3A	2.93	1.62	1.59
2	C	201	COA	C8A-N9A	-2.92	1.32	1.37
2	D	201	COA	C5A-C4A	-2.90	1.33	1.39
2	B	201	COA	CEP-CBP	2.83	1.59	1.53
2	D	201	COA	OAP-CAP	-2.77	1.37	1.42
2	B	201	COA	O3B-C3B	-2.77	1.34	1.44
2	B	201	COA	C5A-C4A	-2.75	1.34	1.39
2	A	201	COA	P3B-O9A	-2.74	1.44	1.54
2	A	201	COA	P2A-O5A	-2.70	1.42	1.55
2	B	201	COA	O2B-C2B	2.70	1.49	1.43
2	C	201	COA	C2A-N1A	-2.66	1.29	1.33
2	D	201	COA	CEP-CBP	2.64	1.59	1.53
2	A	201	COA	C4A-N3A	-2.62	1.29	1.34
2	A	201	COA	P3B-O8A	-2.62	1.45	1.54
2	B	201	COA	C3B-C4B	2.58	1.59	1.52
2	C	201	COA	O4B-C1B	-2.57	1.36	1.42
2	C	201	COA	P1A-O5B	-2.56	1.49	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	COA	CEP-CBP	-2.55	1.48	1.53
2	B	201	COA	CDP-CBP	2.55	1.59	1.53
2	B	201	COA	CCP-CBP	2.54	1.56	1.52
2	D	201	COA	C5A-N7A	-2.51	1.34	1.39
2	D	201	COA	CDP-CBP	2.34	1.58	1.53
2	D	201	COA	C3B-C4B	2.27	1.58	1.52
2	D	201	COA	P3B-O3B	2.26	1.63	1.59
2	C	201	COA	P3B-O9A	-2.25	1.46	1.54
2	C	201	COA	P2A-O5A	-2.22	1.45	1.55
2	A	201	COA	C1B-N9A	2.22	1.52	1.46
2	D	201	COA	O2B-C2B	2.18	1.48	1.43
2	D	201	COA	P2A-O6A	2.18	1.67	1.59
2	A	201	COA	C5P-N4P	-2.17	1.28	1.33
2	B	201	COA	P3B-O3B	2.17	1.63	1.59
2	B	201	COA	C1B-N9A	-2.14	1.40	1.46
2	C	201	COA	O4B-C4B	-2.14	1.40	1.45
2	D	201	COA	C7P-C6P	2.13	1.58	1.51
2	A	201	COA	C8A-N7A	2.10	1.35	1.31

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	COA	CDP-CBP-CAP	9.60	125.13	108.77
2	B	201	COA	N6A-C6A-N1A	-8.56	99.31	118.38
2	D	201	COA	N6A-C6A-N1A	-8.47	99.51	118.38
2	B	201	COA	CAP-C9P-N8P	7.78	131.24	116.48
2	A	201	COA	CEP-CBP-CAP	-7.39	96.17	108.77
2	B	201	COA	C5A-C6A-N6A	7.00	140.62	123.29
2	D	201	COA	C5A-C6A-N6A	6.92	140.42	123.29
2	C	201	COA	CEP-CBP-CAP	-6.71	97.32	108.77
2	D	201	COA	C7P-C6P-C5P	6.53	123.26	112.39
2	C	201	COA	C2B-C3B-C4B	-6.48	91.89	103.24
2	D	201	COA	O6A-CCP-CBP	6.35	120.76	110.55
2	C	201	COA	N3A-C2A-N1A	-6.12	119.32	128.58
2	D	201	COA	N3A-C2A-N1A	-6.02	119.47	128.58
2	B	201	COA	N3A-C2A-N1A	-6.00	119.51	128.58
2	B	201	COA	N9A-C8A-N7A	-5.47	106.17	113.94
2	C	201	COA	O4B-C1B-C2B	-5.18	95.53	106.62
2	C	201	COA	O3B-C3B-C4B	-4.96	92.54	110.03
2	B	201	COA	O9P-C9P-N8P	-4.78	112.87	122.98
2	B	201	COA	O6A-CCP-CBP	-4.78	102.87	110.55
2	A	201	COA	C5A-C4A-N3A	-4.57	120.43	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	COA	CDP-CBP-CCP	4.51	115.67	108.22
2	D	201	COA	N9A-C8A-N7A	-4.46	107.61	113.94
2	B	201	COA	CDP-CBP-CAP	4.42	116.30	108.77
2	A	201	COA	C3P-N4P-C5P	-4.25	114.91	122.82
2	D	201	COA	C5A-C4A-N3A	-4.21	120.93	126.72
2	C	201	COA	CAP-C9P-N8P	4.19	124.44	116.48
2	B	201	COA	C4A-N9A-C8A	4.18	110.13	105.74
2	C	201	COA	C6A-C5A-C4A	-4.06	111.64	117.18
2	C	201	COA	C6P-C5P-N4P	3.98	123.59	116.34
2	D	201	COA	C7P-N8P-C9P	3.97	129.68	122.55
2	C	201	COA	C4A-N9A-C8A	3.95	109.88	105.74
2	C	201	COA	C2A-N3A-C4A	3.90	121.34	111.83
2	B	201	COA	C7P-N8P-C9P	3.83	129.42	122.55
2	C	201	COA	O5P-C5P-C6P	-3.79	115.16	122.02
2	A	201	COA	O6A-CCP-CBP	3.77	116.60	110.55
2	A	201	COA	C7P-N8P-C9P	3.69	129.17	122.55
2	B	201	COA	C5A-C4A-N3A	-3.65	121.69	126.72
2	A	201	COA	CAP-C9P-N8P	3.63	123.36	116.48
2	C	201	COA	C2A-N1A-C6A	3.62	124.67	118.73
2	A	201	COA	CEP-CBP-CDP	-3.62	101.99	109.20
2	D	201	COA	O5P-C5P-N4P	-3.53	116.10	123.03
2	C	201	COA	O3A-P2A-O4A	3.37	120.85	110.70
2	D	201	COA	CDP-CBP-CAP	3.36	114.50	108.77
2	B	201	COA	C5A-N7A-C8A	3.27	108.59	103.45
2	A	201	COA	CEP-CBP-CCP	3.26	113.60	108.22
2	D	201	COA	O2A-P1A-O3A	3.24	116.03	107.27
2	D	201	COA	C2A-N3A-C4A	3.20	119.64	111.83
2	A	201	COA	C7P-C6P-C5P	3.17	117.68	112.39
2	D	201	COA	O3A-P2A-O4A	-3.16	101.21	110.70
2	A	201	COA	C2A-N3A-C4A	3.14	119.50	111.83
2	C	201	COA	C6A-C5A-N7A	3.11	138.09	132.09
2	A	201	COA	O4B-C1B-N9A	3.03	113.90	108.09
2	B	201	COA	C2A-N3A-C4A	3.02	119.20	111.83
2	B	201	COA	CDP-CBP-CCP	-2.98	103.30	108.22
2	A	201	COA	CDP-CBP-CCP	-2.95	103.35	108.22
2	A	201	COA	N3A-C4A-N9A	2.92	132.14	127.17
2	C	201	COA	N3A-C4A-N9A	2.89	132.08	127.17
2	D	201	COA	P3B-O3B-C3B	-2.84	115.86	123.43
2	D	201	COA	C5A-N7A-C8A	2.83	107.90	103.45
2	C	201	COA	O2A-P1A-O3A	2.80	114.83	107.27
2	A	201	COA	O9A-P3B-O7A	2.77	121.63	110.83
2	D	201	COA	CAP-C9P-N8P	2.76	121.71	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	COA	C3P-N4P-C5P	-2.73	117.75	122.82
2	D	201	COA	CEP-CBP-CAP	-2.73	104.12	108.77
2	A	201	COA	O5A-P2A-O3A	-2.71	99.96	107.27
2	C	201	COA	C3B-C2B-C1B	2.69	105.80	99.89
2	C	201	COA	C4A-N9A-C1B	-2.67	120.40	126.63
2	D	201	COA	C1B-N9A-C8A	-2.63	121.27	127.09
2	D	201	COA	OAP-CAP-CBP	-2.60	104.16	110.18
2	C	201	COA	O9P-C9P-CAP	-2.54	113.79	120.89
2	D	201	COA	CEP-CBP-CCP	2.47	112.31	108.22
2	C	201	COA	O9A-P3B-O8A	2.46	117.04	107.80
2	D	201	COA	C4A-N9A-C8A	2.46	108.32	105.74
2	A	201	COA	N3A-C2A-N1A	-2.45	124.87	128.58
2	C	201	COA	C5A-C4A-N3A	-2.43	123.36	126.72
2	B	201	COA	N3A-C4A-N9A	2.39	131.23	127.17
2	B	201	COA	OAP-CAP-CBP	-2.39	104.65	110.18
2	D	201	COA	C6P-C5P-N4P	2.36	120.64	116.34
2	D	201	COA	N3A-C4A-N9A	2.35	131.17	127.17
2	B	201	COA	C1B-N9A-C8A	-2.33	121.93	127.09
2	B	201	COA	CEP-CBP-CCP	-2.33	104.38	108.22
2	B	201	COA	C6P-C5P-N4P	2.24	120.42	116.34
2	B	201	COA	C4A-C5A-N7A	-2.24	108.02	110.58
2	A	201	COA	C6P-C7P-N8P	-2.22	107.27	112.00
2	C	201	COA	N9A-C8A-N7A	-2.22	110.78	113.94
2	A	201	COA	N6A-C6A-N1A	2.22	123.32	118.38
2	A	201	COA	P2A-O6A-CCP	2.21	133.17	121.12
2	A	201	COA	C3B-C2B-C1B	2.20	104.73	99.89
2	B	201	COA	O5P-C5P-N4P	-2.13	118.86	123.03
2	A	201	COA	O3A-P1A-O1A	-2.09	104.41	110.70
2	D	201	COA	C4A-C5A-N7A	-2.01	108.28	110.58

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	COA	C5B-O5B-P1A-O2A
2	B	201	COA	C5B-O5B-P1A-O3A
2	B	201	COA	CCP-O6A-P2A-O3A
2	B	201	COA	CCP-O6A-P2A-O5A
2	B	201	COA	CEP-CBP-CCP-O6A
2	B	201	COA	CAP-CBP-CCP-O6A
2	B	201	COA	OAP-CAP-CBP-CCP
2	B	201	COA	C9P-CAP-CBP-CCP

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Mol	Chain	Res	Type	Atoms
2	B	201	COA	OAP-CAP-CBP-CDP
2	B	201	COA	C9P-CAP-CBP-CDP
2	B	201	COA	OAP-CAP-CBP-CEP
2	B	201	COA	C9P-CAP-CBP-CEP
2	B	201	COA	O9P-C9P-CAP-CBP
2	B	201	COA	N8P-C9P-CAP-CBP
2	B	201	COA	N8P-C9P-CAP-OAP
2	B	201	COA	CAP-C9P-N8P-C7P
2	B	201	COA	S1P-C2P-C3P-N4P
2	A	201	COA	C2B-C1B-N9A-C4A
2	A	201	COA	C4B-C3B-O3B-P3B
2	A	201	COA	C5B-O5B-P1A-O3A
2	A	201	COA	CAP-CBP-CCP-O6A
2	A	201	COA	OAP-CAP-CBP-CCP
2	A	201	COA	C9P-CAP-CBP-CCP
2	A	201	COA	OAP-CAP-CBP-CDP
2	A	201	COA	C9P-CAP-CBP-CDP
2	A	201	COA	OAP-CAP-CBP-CEP
2	A	201	COA	C9P-CAP-CBP-CEP
2	A	201	COA	O9P-C9P-CAP-CBP
2	A	201	COA	N8P-C9P-CAP-CBP
2	A	201	COA	N8P-C9P-CAP-OAP
2	A	201	COA	C6P-C5P-N4P-C3P
2	A	201	COA	O5P-C5P-N4P-C3P
2	A	201	COA	S1P-C2P-C3P-N4P
2	C	201	COA	C4B-C5B-O5B-P1A
2	C	201	COA	CDP-CBP-CCP-O6A
2	C	201	COA	CEP-CBP-CCP-O6A
2	C	201	COA	CAP-CBP-CCP-O6A
2	C	201	COA	OAP-CAP-CBP-CCP
2	C	201	COA	C9P-CAP-CBP-CCP
2	C	201	COA	C9P-CAP-CBP-CEP
2	C	201	COA	O9P-C9P-CAP-CBP
2	C	201	COA	N8P-C9P-CAP-CBP
2	C	201	COA	C6P-C5P-N4P-C3P
2	C	201	COA	O5P-C5P-N4P-C3P
2	C	201	COA	S1P-C2P-C3P-N4P
2	D	201	COA	C5B-O5B-P1A-O2A
2	D	201	COA	C5B-O5B-P1A-O3A
2	D	201	COA	CBP-CCP-O6A-P2A
2	D	201	COA	CDP-CBP-CCP-O6A
2	D	201	COA	CEP-CBP-CCP-O6A

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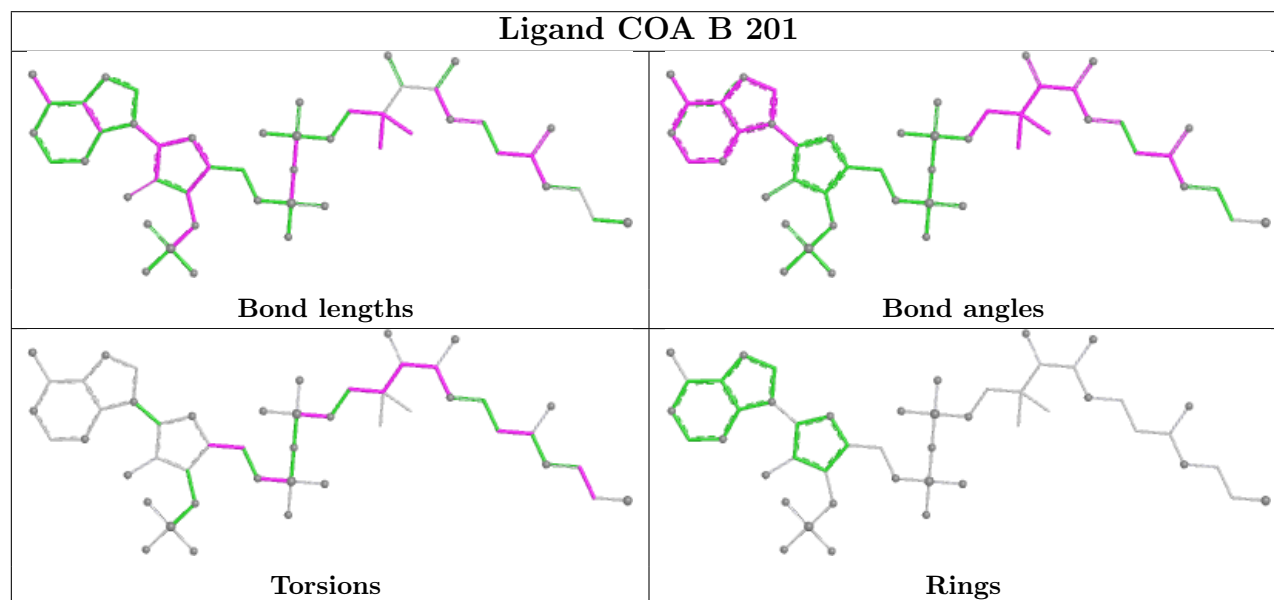
Mol	Chain	Res	Type	Atoms
2	D	201	COA	CAP-CBP-CCP-O6A
2	D	201	COA	OAP-CAP-CBP-CCP
2	D	201	COA	C9P-CAP-CBP-CCP
2	D	201	COA	OAP-CAP-CBP-CDP
2	D	201	COA	C9P-CAP-CBP-CDP
2	D	201	COA	OAP-CAP-CBP-CEP
2	D	201	COA	C9P-CAP-CBP-CEP
2	D	201	COA	O9P-C9P-CAP-CBP
2	D	201	COA	N8P-C9P-CAP-CBP
2	D	201	COA	N8P-C9P-CAP-OAP
2	D	201	COA	C5P-C6P-C7P-N8P
2	D	201	COA	S1P-C2P-C3P-N4P
2	B	201	COA	O9P-C9P-N8P-C7P
2	B	201	COA	O4B-C4B-C5B-O5B
2	A	201	COA	O4B-C4B-C5B-O5B
2	A	201	COA	C3B-C4B-C5B-O5B
2	A	201	COA	C2B-C1B-N9A-C8A
2	A	201	COA	O9P-C9P-CAP-OAP
2	C	201	COA	O9P-C9P-CAP-OAP
2	C	201	COA	C3B-O3B-P3B-O7A
2	A	201	COA	CAP-C9P-N8P-C7P
2	A	201	COA	O9P-C9P-N8P-C7P
2	B	201	COA	C3B-C4B-C5B-O5B
2	D	201	COA	P2A-O3A-P1A-O1A
2	D	201	COA	P1A-O3A-P2A-O5A
2	B	201	COA	CDP-CBP-CCP-O6A
2	A	201	COA	CEP-CBP-CCP-O6A
2	D	201	COA	C2P-C3P-N4P-C5P
2	B	201	COA	C5B-O5B-P1A-O1A
2	B	201	COA	CCP-O6A-P2A-O4A
2	A	201	COA	CCP-O6A-P2A-O4A
2	A	201	COA	C5P-C6P-C7P-N8P
2	D	201	COA	C2B-C1B-N9A-C8A
2	D	201	COA	O4B-C4B-C5B-O5B
2	A	201	COA	C2P-C3P-N4P-C5P
2	B	201	COA	O5P-C5P-C6P-C7P
2	D	201	COA	P1A-O3A-P2A-O4A
2	A	201	COA	C3B-O3B-P3B-O7A
2	A	201	COA	C2B-C3B-O3B-P3B
2	C	201	COA	N8P-C9P-CAP-OAP
2	D	201	COA	P2A-O3A-P1A-O2A

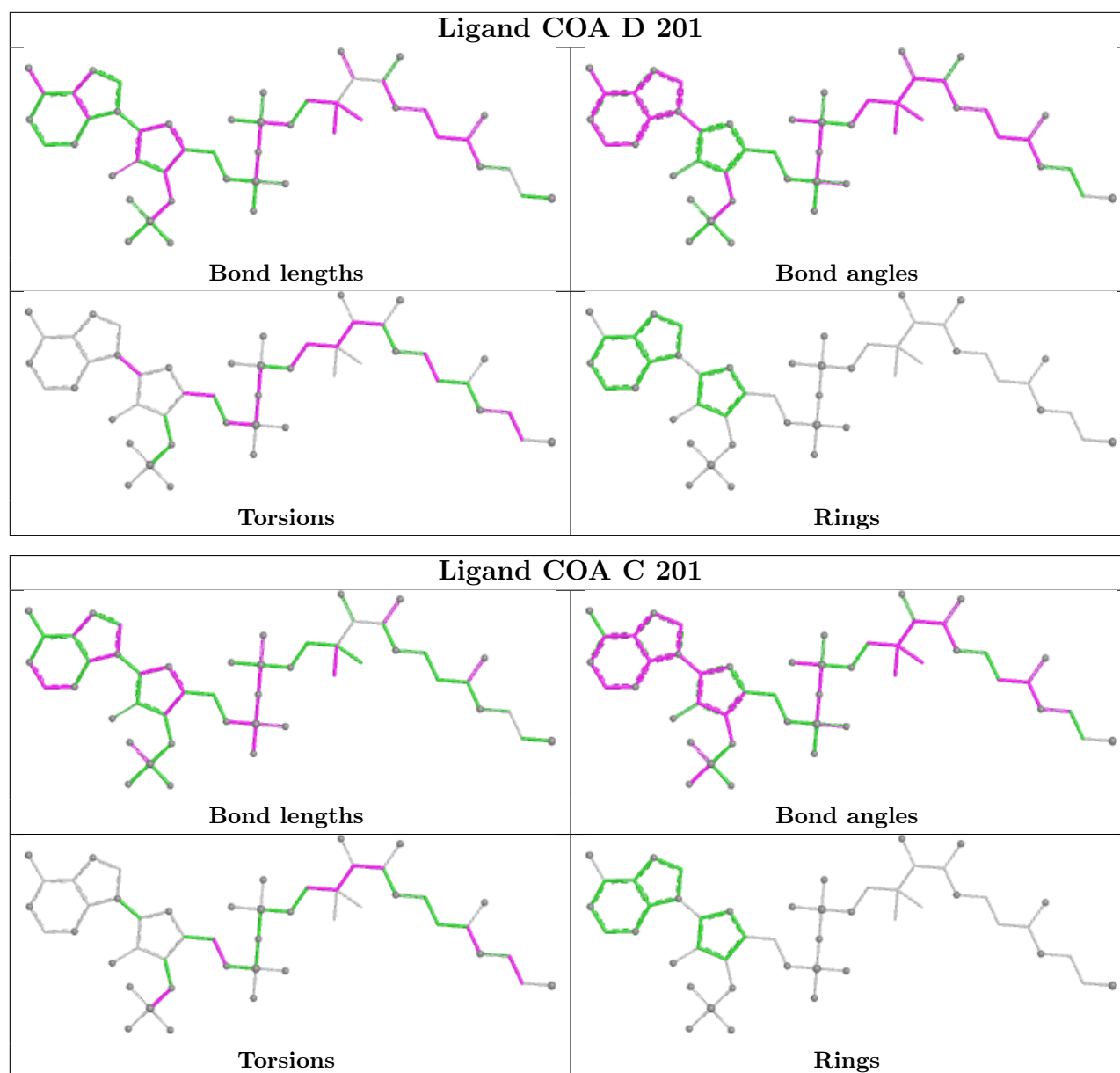
There are no ring outliers.

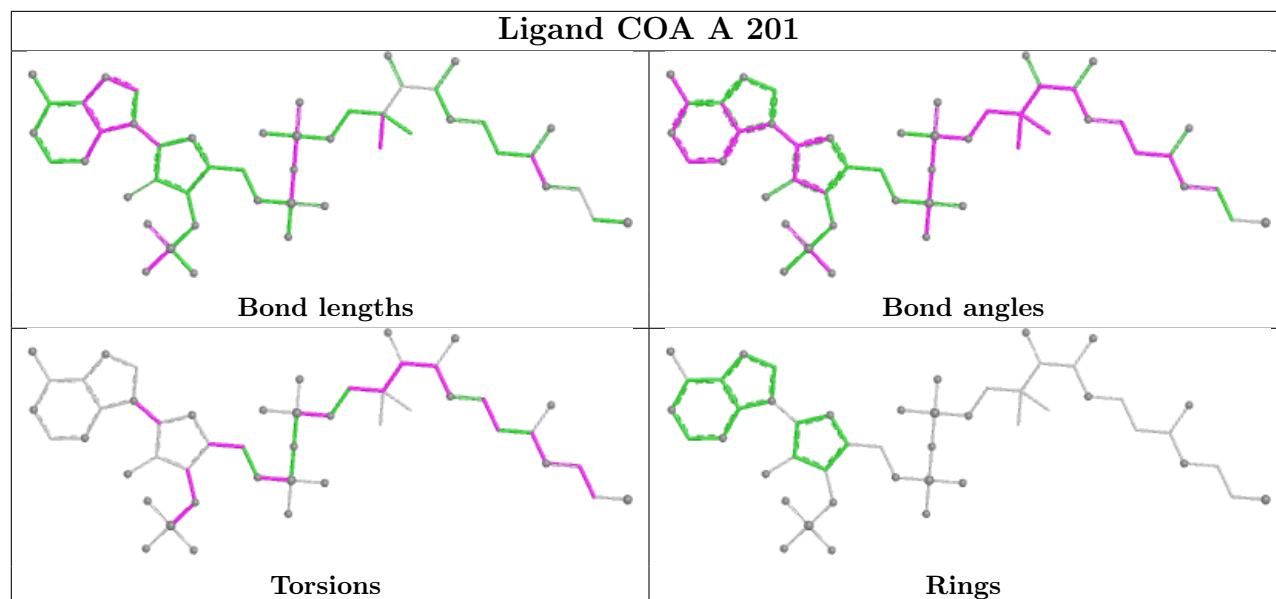
4 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	COA	5	0
2	D	201	COA	11	0
2	C	201	COA	11	0
2	A	201	COA	7	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	187/193 (96%)	0.49	7 (3%)	45 25	13, 26, 41, 55	0
1	B	187/193 (96%)	0.56	11 (5%)	28 14	14, 25, 48, 55	0
1	C	187/193 (96%)	0.57	6 (3%)	50 28	12, 27, 43, 62	0
1	D	187/193 (96%)	0.56	13 (6%)	22 11	13, 26, 46, 58	0
All	All	748/772 (96%)	0.55	37 (4%)	35 17	12, 26, 47, 62	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	48	ASP	3.3
1	B	21	GLU	3.3
1	A	24	LEU	3.1
1	D	70	ASP	2.9
1	C	182	THR	2.9
1	C	186	GLU	2.9
1	C	65	TYR	2.8
1	A	120	GLN	2.8
1	A	65	TYR	2.7
1	B	188	SER	2.6
1	D	65	TYR	2.6
1	B	28	LEU	2.5
1	B	65	TYR	2.5
1	D	33	ALA	2.5
1	D	135	LEU	2.5
1	D	160	ASP	2.4
1	A	160	ASP	2.4
1	D	2	PHE	2.4
1	D	47	PRO	2.4
1	D	151	GLN	2.3
1	C	46	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	5	GLN	2.3
1	B	36	GLN	2.3
1	C	181	ARG	2.3
1	D	98	GLU	2.3
1	A	185	THR	2.3
1	B	29	SER	2.2
1	D	25	VAL	2.2
1	D	3	LYS	2.2
1	A	187	LEU	2.2
1	B	143	LYS	2.1
1	B	48	ASP	2.1
1	D	136	ARG	2.1
1	B	182	THR	2.1
1	B	43	GLY	2.1
1	A	186	GLU	2.1
1	D	188	SER	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.

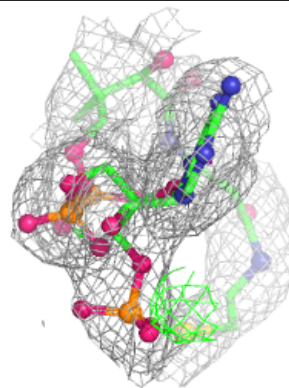
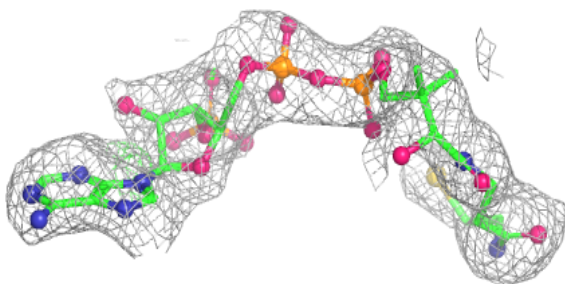
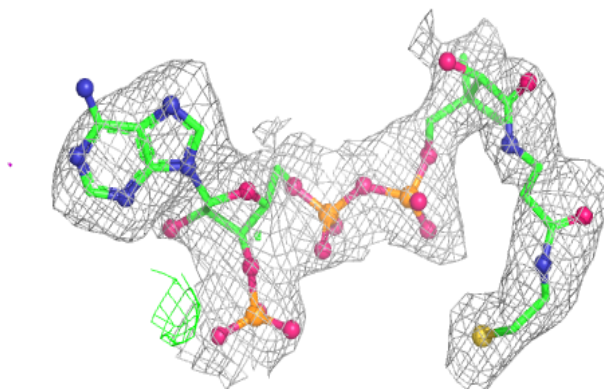
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	COA	C	201	48/48	0.82	0.15	22,40,52,63	0
2	COA	A	201	48/48	0.84	0.15	26,49,68,78	0
2	COA	B	201	48/48	0.90	0.12	14,29,44,49	0
2	COA	D	201	48/48	0.90	0.13	15,28,38,43	0

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.

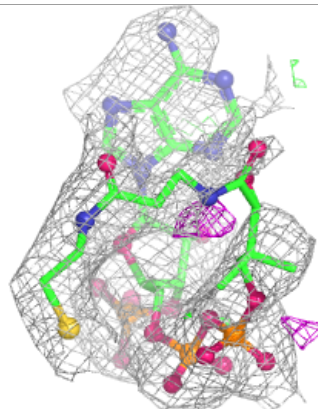
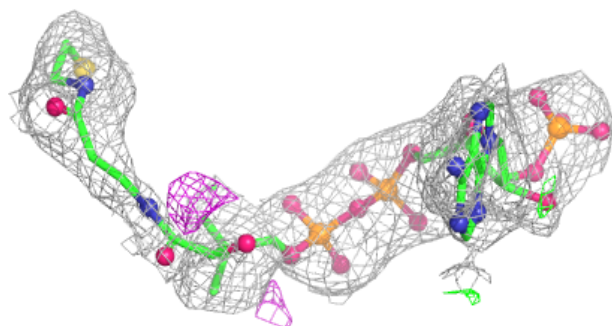
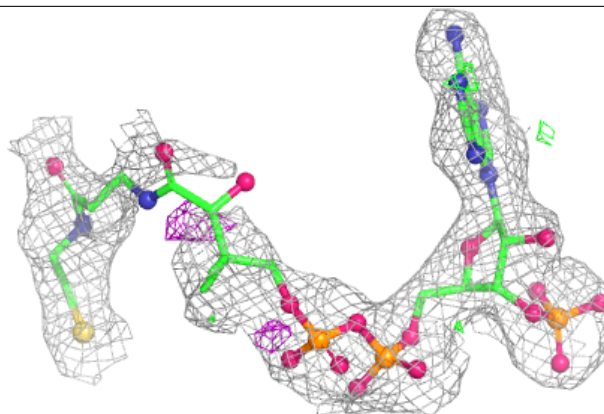
Electron density around COA C 201:

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



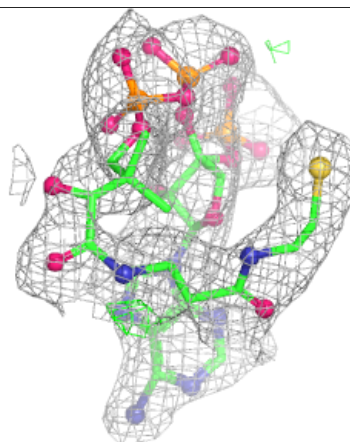
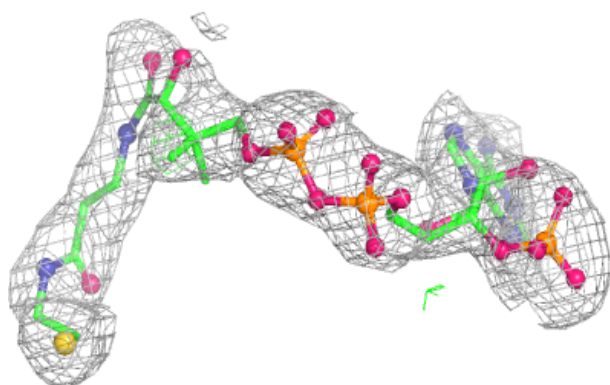
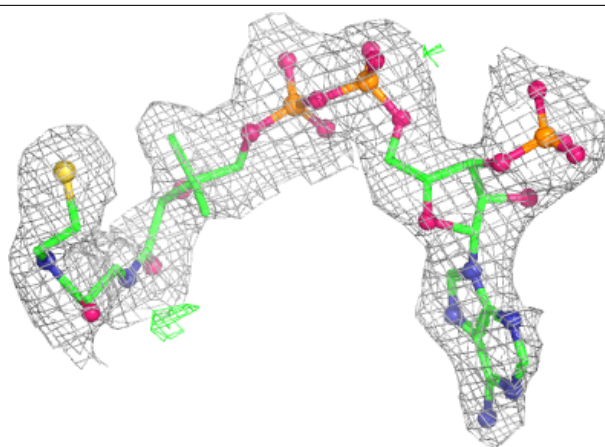
Electron density around COA A 201:

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

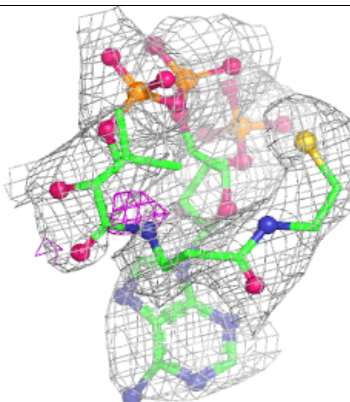
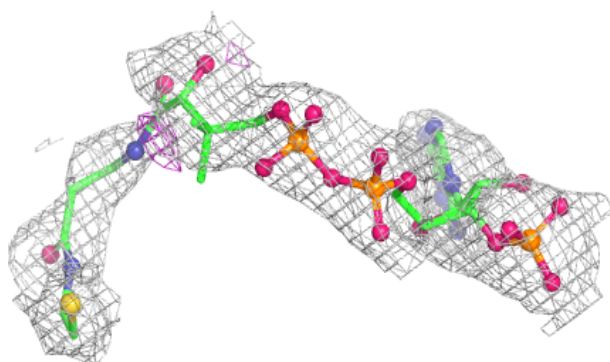
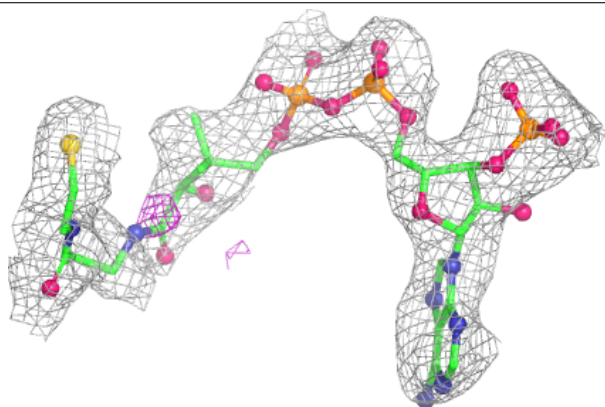


Electron density around COA B 201:

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

**Electron density around COA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.