



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:49 PM UTC

PDB ID : 1LY3 / pdb_00001ly3
Title : ANALYSIS OF QUINAZOLINE AND PYRIDOPYRIMIDINE N9-C10 REVERSED BRIDGE ANTIFOLATES IN COMPLEX WITH NADP⁺ AND PNEUMOCYSTIS CARINII DIHYDROFOLATE REDUCTASE
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Deposited on : 2002-06-06
Resolution : 1.90 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

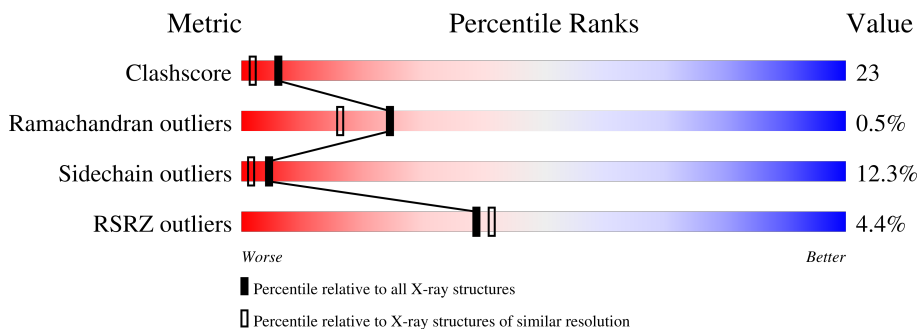
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	206	

2 Entry composition [i](#)

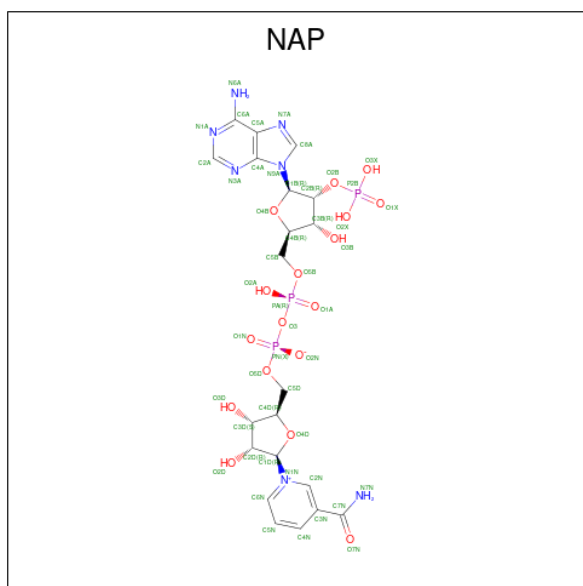
There are 4 unique types of molecules in this entry. The entry contains 1836 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIHYDROFOLATE REDUCTASE.

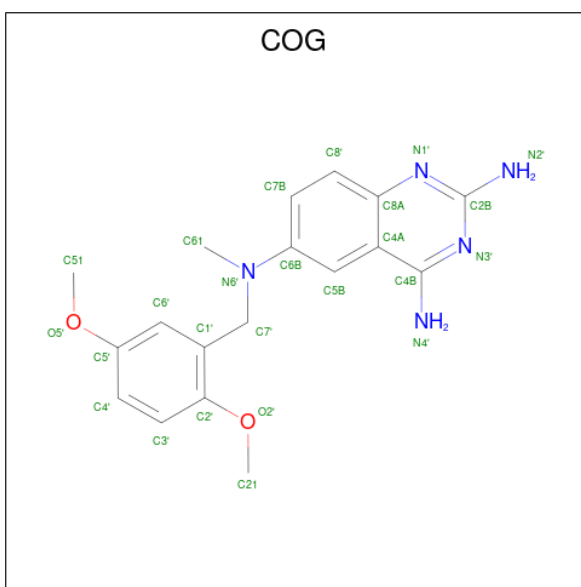
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	206	1686	1086	288	305	7	0	0	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0

- Molecule 3 is 2,4-DIAMINO-6-[N-(2',5'-DIMETHOXYBENZYL)-N-METHYLAMINO]QUINAZOLINE (CCD ID: COG) (formula: $C_{18}H_{21}N_5O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	18	5	2		

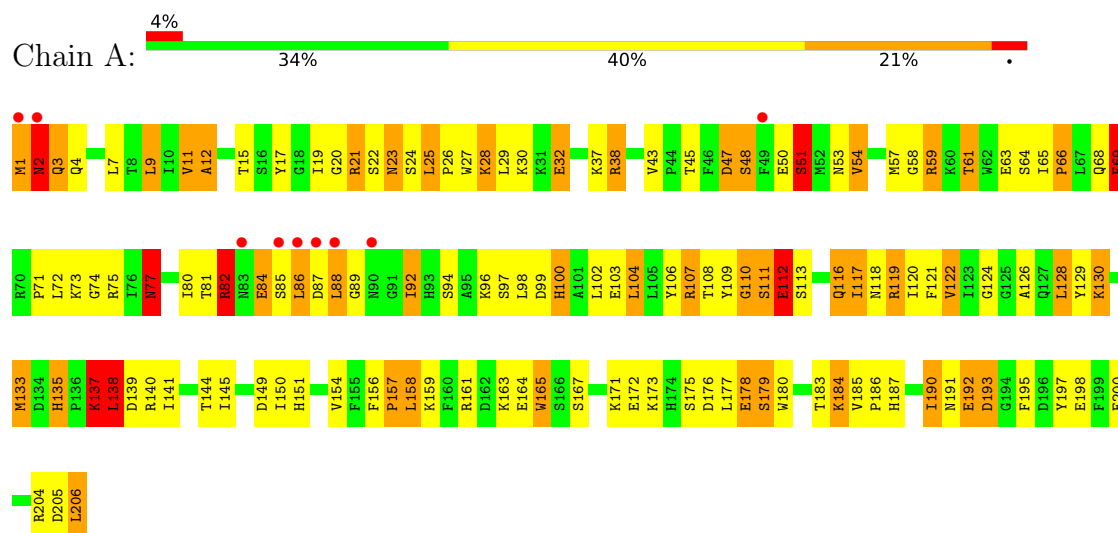
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	77	Total	O	0	0
			77	77		

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: DIHYDROFOLATE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	37.37Å 43.26Å 61.37Å 90.00° 94.77° 90.00°	Depositor
Resolution (Å)	8.00 – 1.90 8.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.3 (8.00-1.90) 84.0 (8.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.52 (at 1.89Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.178 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 84.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1836	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.72% 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: COG, NAP

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	1.44	9/1728 (0.5%)	2.56	146/2330 (6.3%)

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	A	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	SER	C-N	11.92	1.50	1.33
1	A	87	ASP	C-N	-11.28	1.17	1.33
1	A	66	PRO	C-N	6.30	1.42	1.33
1	A	122	VAL	C-O	6.20	1.30	1.24
1	A	180	TRP	C-N	-6.14	1.28	1.34
1	A	129	TYR	C-N	-5.95	1.26	1.33
1	A	69	PHE	C-N	-5.70	1.26	1.33
1	A	110	GLY	N-CA	5.70	1.49	1.44
1	A	73	LYS	CA-CB	5.34	1.61	1.53

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ARG	CD-NE-CZ	17.25	148.56	124.40
1	A	21	ARG	CD-NE-CZ	11.40	140.36	124.40
1	A	85	SER	N-CA-C	-10.36	97.35	111.96
1	A	140	ARG	NE-CZ-NH1	9.88	131.38	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	MET	CA-C-N	9.77	131.57	120.53
1	A	57	MET	C-N-CA	9.77	131.57	120.53
1	A	84	GLU	N-CA-C	-9.73	95.14	109.15
1	A	99	ASP	CA-CB-CG	-9.35	103.25	112.60
1	A	87	ASP	CA-CB-CG	9.24	121.84	112.60
1	A	198	GLU	N-CA-CB	-9.05	94.68	111.52
1	A	140	ARG	NH1-CZ-NH2	-9.04	107.55	119.30
1	A	37	LYS	CA-C-N	8.69	131.73	120.44
1	A	37	LYS	C-N-CA	8.69	131.73	120.44
1	A	165	TRP	CA-C-O	-8.46	109.66	119.56
1	A	107	ARG	CD-NE-CZ	8.38	136.13	124.40
1	A	53	ASN	OD1-CG-ND2	-8.36	114.24	122.60
1	A	138	LEU	CB-CA-C	7.91	123.98	110.77
1	A	59	ARG	CA-C-O	-7.86	112.09	120.42
1	A	48	SER	CA-C-N	-7.71	108.58	121.92
1	A	48	SER	C-N-CA	-7.71	108.58	121.92
1	A	99	ASP	O-C-N	7.64	131.66	122.27
1	A	61	THR	CA-CB-OG1	-7.49	98.36	109.60
1	A	82	ARG	CA-C-O	7.48	129.12	120.00
1	A	23	ASN	CA-C-O	7.38	130.30	121.08
1	A	107	ARG	NE-CZ-NH1	-7.30	114.20	121.50
1	A	66	PRO	O-C-N	7.10	131.91	122.89
1	A	77	ASN	O-C-N	7.02	131.20	123.27
1	A	135	HIS	CA-C-O	7.01	126.81	119.80
1	A	176	ASP	CA-CB-CG	-6.96	105.64	112.60
1	A	157	PRO	N-CA-C	6.91	122.50	113.86
1	A	48	SER	O-C-N	-6.80	113.55	122.39
1	A	15	THR	CA-CB-OG1	-6.79	99.41	109.60
1	A	85	SER	CB-CA-C	6.79	122.89	110.88
1	A	87	ASP	N-CA-C	-6.76	97.71	108.73
1	A	77	ASN	CA-CB-CG	6.71	119.31	112.60
1	A	22	SER	CA-C-N	6.69	131.92	122.08
1	A	22	SER	C-N-CA	6.69	131.92	122.08
1	A	92	ILE	O-C-N	6.69	130.93	123.10
1	A	158	LEU	CB-CA-C	6.68	121.33	109.65
1	A	133	MET	O-C-N	6.67	129.19	122.12
1	A	180	TRP	CA-C-N	6.66	131.79	121.34
1	A	180	TRP	C-N-CA	6.66	131.79	121.34
1	A	58	GLY	N-CA-C	-6.64	104.03	112.54
1	A	92	ILE	N-CA-C	-6.63	98.18	107.80
1	A	21	ARG	CA-CB-CG	6.55	127.19	114.10
1	A	112	GLU	CA-CB-CG	6.49	127.08	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ALA	N-CA-CB	6.48	120.76	110.65
1	A	118	ASN	CB-CG-ND2	6.48	126.11	116.40
1	A	109	TYR	N-CA-C	6.45	118.38	109.54
1	A	124	GLY	CA-C-O	-6.45	117.10	122.33
1	A	32	GLU	N-CA-C	-6.44	104.34	111.36
1	A	205	ASP	CA-CB-CG	6.44	119.04	112.60
1	A	37	LYS	O-C-N	-6.43	115.40	122.09
1	A	119	ARG	NE-CZ-NH1	6.43	127.93	121.50
1	A	38	ARG	CA-CB-CG	6.41	126.91	114.10
1	A	116	GLN	OE1-CD-NE2	-6.41	116.19	122.60
1	A	85	SER	CA-C-O	6.37	129.85	120.42
1	A	198	GLU	CG-CD-OE2	-6.34	103.81	118.40
1	A	94	SER	CA-C-O	-6.33	113.86	120.70
1	A	72	LEU	CA-C-N	6.29	130.49	121.50
1	A	72	LEU	C-N-CA	6.29	130.49	121.50
1	A	51	SER	N-CA-C	6.24	120.09	110.42
1	A	119	ARG	NE-CZ-NH2	-6.18	113.64	119.20
1	A	204	ARG	NE-CZ-NH1	-6.17	115.33	121.50
1	A	144	THR	CA-CB-OG1	-6.15	100.38	109.60
1	A	75	ARG	NE-CZ-NH1	6.10	127.60	121.50
1	A	192	GLU	CA-C-O	-6.09	112.72	120.27
1	A	54	VAL	CA-C-O	-6.07	113.80	120.72
1	A	86	LEU	CB-CA-C	6.04	118.67	110.94
1	A	9	LEU	CA-C-O	-6.02	114.11	120.80
1	A	72	LEU	CB-CA-C	5.98	119.22	109.90
1	A	21	ARG	CG-CD-NE	5.95	125.09	112.00
1	A	87	ASP	CA-C-N	5.94	129.99	121.50
1	A	87	ASP	C-N-CA	5.94	129.99	121.50
1	A	2	ASN	OD1-CG-ND2	5.93	128.53	122.60
1	A	133	MET	CA-C-O	-5.92	114.27	120.55
1	A	179	SER	N-CA-CB	5.90	118.57	110.01
1	A	108	THR	CA-C-O	-5.90	112.12	119.38
1	A	151	HIS	CA-CB-CG	-5.89	107.91	113.80
1	A	149	ASP	CA-CB-CG	5.88	118.48	112.60
1	A	20	GLY	CA-C-O	-5.88	115.86	121.62
1	A	158	LEU	N-CA-CB	-5.85	100.98	110.81
1	A	198	GLU	CG-CD-OE1	5.81	131.76	118.40
1	A	43	VAL	O-C-N	5.79	127.70	121.10
1	A	25	LEU	CA-C-O	5.74	125.75	119.32
1	A	11	VAL	N-CA-C	5.69	116.56	108.42
1	A	187	HIS	CA-C-O	-5.67	115.03	121.72
1	A	7	LEU	CA-C-O	-5.65	114.72	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ASP	O-C-N	5.62	130.06	122.59
1	A	121	PHE	N-CA-C	5.57	117.98	108.90
1	A	178	GLU	CA-C-O	-5.57	114.64	120.55
1	A	141	ILE	O-C-N	5.52	128.92	123.18
1	A	43	VAL	CA-C-O	-5.51	112.57	119.95
1	A	73	LYS	N-CA-C	5.50	118.50	109.76
1	A	53	ASN	CB-CG-ND2	5.49	124.64	116.40
1	A	111	SER	CA-C-N	5.49	132.00	122.56
1	A	111	SER	C-N-CA	5.49	132.00	122.56
1	A	173	LYS	CB-CA-C	-5.49	99.93	109.64
1	A	191	ASN	CB-CA-C	5.48	119.73	109.71
1	A	150	ILE	O-C-N	5.46	129.18	122.95
1	A	139	ASP	CB-CG-OD1	5.45	130.93	118.40
1	A	32	GLU	N-CA-CB	5.44	118.21	110.16
1	A	197	TYR	CA-C-O	5.44	127.20	121.33
1	A	205	ASP	CB-CG-OD1	5.42	130.87	118.40
1	A	38	ARG	N-CA-CB	-5.41	102.16	110.01
1	A	161	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	A	86	LEU	CA-C-N	-5.39	115.60	122.77
1	A	86	LEU	C-N-CA	-5.39	115.60	122.77
1	A	141	ILE	CA-C-O	-5.38	114.84	120.27
1	A	81	THR	CA-C-O	-5.37	114.09	120.43
1	A	92	ILE	CA-C-O	-5.37	114.78	120.53
1	A	89	GLY	O-C-N	5.34	129.64	122.70
1	A	159	LYS	CG-CD-CE	5.31	123.52	111.30
1	A	87	ASP	CB-CA-C	5.31	118.79	110.19
1	A	117	ILE	CA-CB-CG1	-5.31	101.38	110.40
1	A	167	SER	N-CA-C	-5.31	106.85	113.38
1	A	15	THR	CA-C-N	5.30	131.12	122.65
1	A	15	THR	C-N-CA	5.30	131.12	122.65
1	A	156	PHE	CB-CA-C	5.26	118.35	109.67
1	A	133	MET	N-CA-CB	5.25	117.84	110.12
1	A	63	GLU	CG-CD-OE2	-5.25	106.33	118.40
1	A	172	GLU	CA-C-N	5.22	128.50	120.82
1	A	172	GLU	C-N-CA	5.22	128.50	120.82
1	A	98	LEU	CB-CA-C	5.21	119.07	110.88
1	A	156	PHE	N-CA-C	-5.20	101.85	109.50
1	A	180	TRP	O-C-N	-5.20	116.61	122.12
1	A	74	GLY	O-C-N	5.19	128.90	122.41
1	A	94	SER	CA-CB-OG	5.14	121.37	111.10
1	A	144	THR	CA-C-O	-5.12	114.69	120.32
1	A	135	HIS	CA-CB-CG	-5.11	108.69	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ILE	CA-C-N	-5.11	115.78	122.99
1	A	190	ILE	C-N-CA	-5.11	115.78	122.99
1	A	130	LYS	CA-CB-CG	5.11	124.32	114.10
1	A	137	LYS	N-CA-CB	5.09	118.12	110.53
1	A	145	ILE	CA-C-O	-5.09	114.69	120.65
1	A	159	LYS	CA-C-N	5.07	127.58	120.28
1	A	159	LYS	C-N-CA	5.07	127.58	120.28
1	A	100	HIS	CA-CB-CG	-5.06	108.74	113.80
1	A	47	ASP	CB-CA-C	-5.06	101.63	110.17
1	A	17	TYR	CA-CB-CG	-5.05	104.80	113.90
1	A	161	ARG	NH1-CZ-NH2	-5.04	112.75	119.30
1	A	57	MET	CA-C-O	-5.03	115.23	121.06
1	A	138	LEU	CA-C-N	-5.02	114.11	122.08
1	A	138	LEU	C-N-CA	-5.02	114.11	122.08
1	A	175	SER	CA-CB-OG	5.01	121.12	111.10
1	A	65	ILE	O-C-N	5.00	127.32	121.57

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	69	PHE	Mainchain

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	1686	0	1692	78	1
2	A	48	0	25	4	0
3	A	25	0	21	2	0
4	A	77	0	0	5	0
All	All	1836	0	1738	79	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 23.

All (79) 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:A:82:ARG:HG3	1:A:82:ARG:HH11	1.09	1.13
1:A:82:ARG:HG3	1:A:82:ARG:NH1	1.69	0.89
1:A:104:LEU:C	1:A:104:LEU:HD12	2.00	0.87
1:A:28:LYS:HG2	1:A:28:LYS:O	1.71	0.86
1:A:104:LEU:HD12	1:A:104:LEU:O	1.76	0.85
1:A:66:PRO:HB2	1:A:69:PHE:CD2	2.13	0.83
1:A:82:ARG:HH11	1:A:82:ARG:CG	1.88	0.82
1:A:23:ASN:HD22	2:A:207:NAP:H3D	1.47	0.80
1:A:23:ASN:ND2	2:A:207:NAP:H3D	1.97	0.79
1:A:66:PRO:HB2	1:A:69:PHE:HD2	1.49	0.75
1:A:135:HIS:HD2	1:A:137:LYS:H	1.31	0.75
1:A:84:GLU:O	1:A:84:GLU:OE1	2.05	0.75
1:A:117:ILE:HG21	1:A:120:ILE:HD11	1.67	0.74
1:A:28:LYS:O	1:A:28:LYS:CG	2.37	0.72
1:A:112:GLU:O	1:A:112:GLU:OE2	2.07	0.72
1:A:26:PRO:HG2	1:A:27:TRP:CE3	2.25	0.71
1:A:171:LYS:NZ	1:A:200:GLU:OE2	2.26	0.68
1:A:54:VAL:HG21	1:A:117:ILE:HD13	1.77	0.67
1:A:107:ARG:HG2	4:A:220:HOH:O	1.97	0.65
1:A:130:LYS:HG2	1:A:157:PRO:HB3	1.78	0.64
1:A:88:LEU:C	1:A:88:LEU:HD23	2.22	0.64
1:A:117:ILE:CG2	1:A:120:ILE:HD11	2.28	0.64
1:A:96:LYS:HE2	1:A:100:HIS:CE1	2.32	0.63
1:A:1:MET:HA	1:A:1:MET:HE2	1.81	0.63
1:A:135:HIS:CD2	1:A:137:LYS:H	2.15	0.62
1:A:122:VAL:HG13	1:A:128:LEU:HD13	1.82	0.60
1:A:84:GLU:O	1:A:84:GLU:CD	2.45	0.60
1:A:177:LEU:C	1:A:177:LEU:HD23	2.27	0.60
1:A:186:PRO:HB2	1:A:190:ILE:HD11	1.85	0.59
1:A:164:GLU:HG3	1:A:165:TRP:CD1	2.38	0.58
1:A:45:THR:HA	1:A:48:SER:OG	2.02	0.58
1:A:50:GLU:HG2	1:A:51:SER:N	2.20	0.56
1:A:3:GLN:HA	1:A:106:TYR:HE2	1.70	0.56
1:A:71:PRO:HG3	1:A:92:ILE:HD11	1.89	0.55
1:A:104:LEU:C	1:A:104:LEU:CD1	2.73	0.55
1:A:126:ALA:HB2	1:A:154:VAL:CG1	2.37	0.55
1:A:192:GLU:O	1:A:193:ASP:HB2	2.07	0.55
1:A:29:LEU:HD11	1:A:195:PHE:CD1	2.43	0.54
1:A:88:LEU:HA	4:A:247:HOH:O	2.08	0.53
1:A:110:GLY:O	1:A:113:SER:N	2.40	0.53
1:A:9:LEU:HB2	1:A:138:LEU:HD21	1.91	0.53
1:A:185:VAL:HG13	1:A:186:PRO:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:THR:O	1:A:64:SER:HB2	2.09	0.52
1:A:130:LYS:HG2	1:A:157:PRO:CB	2.40	0.52
1:A:185:VAL:CG1	1:A:186:PRO:HD2	2.40	0.51
1:A:133:MET:CE	1:A:158:LEU:HD22	2.42	0.50
1:A:66:PRO:CB	1:A:69:PHE:HD2	2.21	0.50
1:A:19:ILE:O	2:A:207:NAP:H2N	2.12	0.50
1:A:69:PHE:CB	3:A:307:COG:H513	2.42	0.50
1:A:178:GLU:HG2	1:A:184:LYS:HA	1.94	0.50
1:A:2:ASN:O	1:A:102:LEU:HB3	2.14	0.48
1:A:47:ASP:HA	1:A:50:GLU:OE2	2.14	0.48
1:A:185:VAL:HA	1:A:186:PRO:HD3	1.79	0.47
1:A:119:ARG:C	1:A:120:ILE:HD13	2.39	0.47
1:A:3:GLN:HA	1:A:106:TYR:CE2	2.50	0.47
1:A:77:ASN:N	1:A:77:ASN:HD22	2.11	0.47
1:A:107:ARG:CG	4:A:220:HOH:O	2.59	0.47
1:A:54:VAL:HB	1:A:120:ILE:HD12	1.96	0.47
1:A:171:LYS:HZ2	1:A:200:GLU:CD	2.22	0.47
1:A:82:ARG:C	1:A:84:GLU:H	2.23	0.47
3:A:307:COG:H5'	3:A:307:COG:H612	1.57	0.47
1:A:19:ILE:HD11	1:A:126:ALA:HB2	1.97	0.47
1:A:103:GLU:CG	4:A:253:HOH:O	2.64	0.45
1:A:2:ASN:O	1:A:106:TYR:CE2	2.69	0.45
1:A:110:GLY:O	1:A:112:GLU:N	2.50	0.45
1:A:2:ASN:O	1:A:106:TYR:HE2	2.00	0.44
1:A:29:LEU:HB3	1:A:32:GLU:HB2	1.98	0.44
1:A:113:SER:O	1:A:116:GLN:NE2	2.49	0.44
1:A:11:VAL:HG22	1:A:12:ALA:N	2.34	0.43
1:A:80:ILE:O	2:A:207:NAP:H1B	2.19	0.43
1:A:84:GLU:HG2	4:A:249:HOH:O	2.18	0.42
1:A:66:PRO:C	1:A:68:GLN:N	2.75	0.42
1:A:178:GLU:HG2	1:A:185:VAL:H	1.85	0.42
1:A:137:LYS:HA	1:A:137:LYS:HE2	2.02	0.42
1:A:133:MET:HE3	1:A:158:LEU:HD22	2.01	0.41
1:A:97:SER:OG	1:A:100:HIS:HD2	2.03	0.41
1:A:25:LEU:HA	1:A:26:PRO:HD2	1.85	0.40
1:A:86:LEU:HD12	1:A:86:LEU:O	2.21	0.40
1:A:137:LYS:HA	1:A:137:LYS:CE	2.51	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:A:163:LYS:NZ	1:A:206:LEU:O[2_546]	1.84	0.36

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	204/206 (99%)	191 (94%)	12 (6%)	1 (0%)	24 16

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	187/187 (100%)	164 (88%)	23 (12%)	4 1

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ASN
1	A	3	GLN
1	A	4	GLN
1	A	21	ARG

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Mol	Chain	Res	Type
1	A	24	SER
1	A	28	LYS
1	A	30	LYS
1	A	38	ARG
1	A	51	SER
1	A	59	ARG
1	A	77	ASN
1	A	82	ARG
1	A	88	LEU
1	A	104	LEU
1	A	112	GLU
1	A	128	LEU
1	A	137	LYS
1	A	138	LEU
1	A	179	SER
1	A	183	THR
1	A	184	LYS
1	A	206	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	23	ASN
1	A	68	GLN
1	A	83	ASN
1	A	100	HIS
1	A	135	HIS
1	A	151	HIS
1	A	187	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

2 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	NAP	A	207	-	50,52,52	3.29	22 (44%)	71,80,80	2.97	25 (35%)
3	COG	A	307	-	27,27,27	1.60	4 (14%)	36,38,38	3.21	14 (38%)

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	NAP	A	207	-	-	6/35/67/67	0/5/5/5
3	COG	A	307	-	-	4/12/12/12	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	207	NAP	C4N-C3N	9.79	1.54	1.39
2	A	207	NAP	P2B-O2B	9.39	1.76	1.59
2	A	207	NAP	O4B-C4B	-8.00	1.27	1.45
2	A	207	NAP	C5N-C4N	6.43	1.49	1.38
2	A	207	NAP	C2N-N1N	5.63	1.41	1.35
2	A	207	NAP	C5A-C6A	5.59	1.56	1.41
2	A	207	NAP	O4D-C1D	4.19	1.46	1.40
2	A	207	NAP	C3B-C4B	4.15	1.63	1.53
3	A	307	COG	C4B-C4A	-4.13	1.41	1.45
2	A	207	NAP	C5A-C4A	-4.04	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	207	NAP	O3B-C3B	3.80	1.52	1.43
3	A	307	COG	C2B-N2'	3.77	1.41	1.33
3	A	307	COG	C2B-N3'	3.63	1.41	1.35
2	A	207	NAP	C5A-N7A	3.52	1.45	1.39
2	A	207	NAP	C4A-N9A	-3.18	1.31	1.37
2	A	207	NAP	C6N-C5N	-3.13	1.32	1.38
2	A	207	NAP	C7N-N7N	2.99	1.38	1.33
2	A	207	NAP	P2B-O2X	-2.93	1.43	1.54
2	A	207	NAP	PN-O1N	-2.91	1.40	1.50
2	A	207	NAP	O7N-C7N	-2.66	1.19	1.24
2	A	207	NAP	O4D-C4D	2.59	1.50	1.45
2	A	207	NAP	PA-O5B	2.58	1.69	1.59
2	A	207	NAP	PA-O2A	-2.45	1.44	1.55
2	A	207	NAP	C6N-N1N	2.36	1.40	1.35
3	A	307	COG	C4B-N4'	2.06	1.41	1.34
2	A	207	NAP	PN-O2N	-2.01	1.46	1.55

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	207	NAP	C5N-C4N-C3N	-11.71	108.86	120.36
3	A	307	COG	C21-O2'-C2'	11.38	134.21	117.51
2	A	207	NAP	O7N-C7N-N7N	8.88	135.45	122.62
2	A	207	NAP	O7N-C7N-C3N	-7.83	110.02	119.60
2	A	207	NAP	O2A-PA-O3	6.48	124.80	107.27
2	A	207	NAP	C2N-C3N-C4N	5.93	125.16	118.26
2	A	207	NAP	C4D-O4D-C1D	-5.75	104.66	109.92
3	A	307	COG	N1'-C2B-N3'	-5.66	120.01	127.21
3	A	307	COG	C61-N6'-C6B	-5.59	110.33	119.59
2	A	207	NAP	O3X-P2B-O2X	5.23	127.39	107.80
3	A	307	COG	O2'-C2'-C1'	4.75	123.03	115.96
3	A	307	COG	C61-N6'-C7'	4.74	127.44	115.11
3	A	307	COG	C51-O5'-C5'	4.39	126.92	117.50
3	A	307	COG	C7B-C6B-N6'	4.26	127.53	121.59
2	A	207	NAP	C6N-C5N-C4N	4.06	125.30	119.45
2	A	207	NAP	O2B-P2B-O1X	-3.85	95.60	109.33
2	A	207	NAP	O3B-C3B-C4B	-3.84	100.04	111.08
3	A	307	COG	C1'-C7'-N6'	-3.76	108.84	114.49
3	A	307	COG	O2'-C2'-C3'	-3.70	118.07	124.30
3	A	307	COG	C7B-C8'-C8A	-3.58	116.52	120.80
3	A	307	COG	C5B-C4A-C4B	-3.40	121.68	124.75
2	A	207	NAP	O4B-C1B-C2B	-3.01	101.41	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	207	NAP	O2D-C2D-C3D	-2.96	102.32	111.82
2	A	207	NAP	C3B-C2B-C1B	-2.93	97.20	102.81
2	A	207	NAP	C2B-C3B-C4B	-2.92	95.71	101.99
2	A	207	NAP	C4B-O4B-C1B	2.77	115.58	109.47
2	A	207	NAP	O5B-PA-O1A	-2.74	98.09	108.94
2	A	207	NAP	C5B-C4B-C3B	-2.63	105.74	115.21
2	A	207	NAP	C3N-C7N-N7N	-2.61	114.53	117.74
3	A	307	COG	C8'-C8A-C4A	2.51	121.84	119.13
2	A	207	NAP	O5D-C5D-C4D	-2.50	100.48	108.99
3	A	307	COG	C6B-C5B-C4A	-2.38	118.97	121.19
2	A	207	NAP	O2B-C2B-C3B	2.35	120.10	111.68
2	A	207	NAP	O5B-C5B-C4B	-2.32	101.10	108.99
2	A	207	NAP	C4A-N9A-C8A	2.30	108.15	105.74
2	A	207	NAP	O3-PA-O1A	-2.20	104.10	110.70
2	A	207	NAP	O2X-P2B-O1X	2.18	119.34	110.83
2	A	207	NAP	O3X-P2B-O1X	-2.02	102.95	110.83
3	A	307	COG	C6'-C1'-C2'	2.01	120.46	118.26

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	207	NAP	O4D-C1D-N1N-C6N
3	A	307	COG	C3'-C2'-O2'-C21
3	A	307	COG	C1'-C2'-O2'-C21
3	A	307	COG	C5B-C6B-N6'-C61
3	A	307	COG	C7B-C6B-N6'-C61
2	A	207	NAP	O4D-C1D-N1N-C2N
2	A	207	NAP	PN-O3-PA-O2A
2	A	207	NAP	C2B-O2B-P2B-O3X
2	A	207	NAP	C1B-C2B-O2B-P2B
2	A	207	NAP	PN-O3-PA-O1A

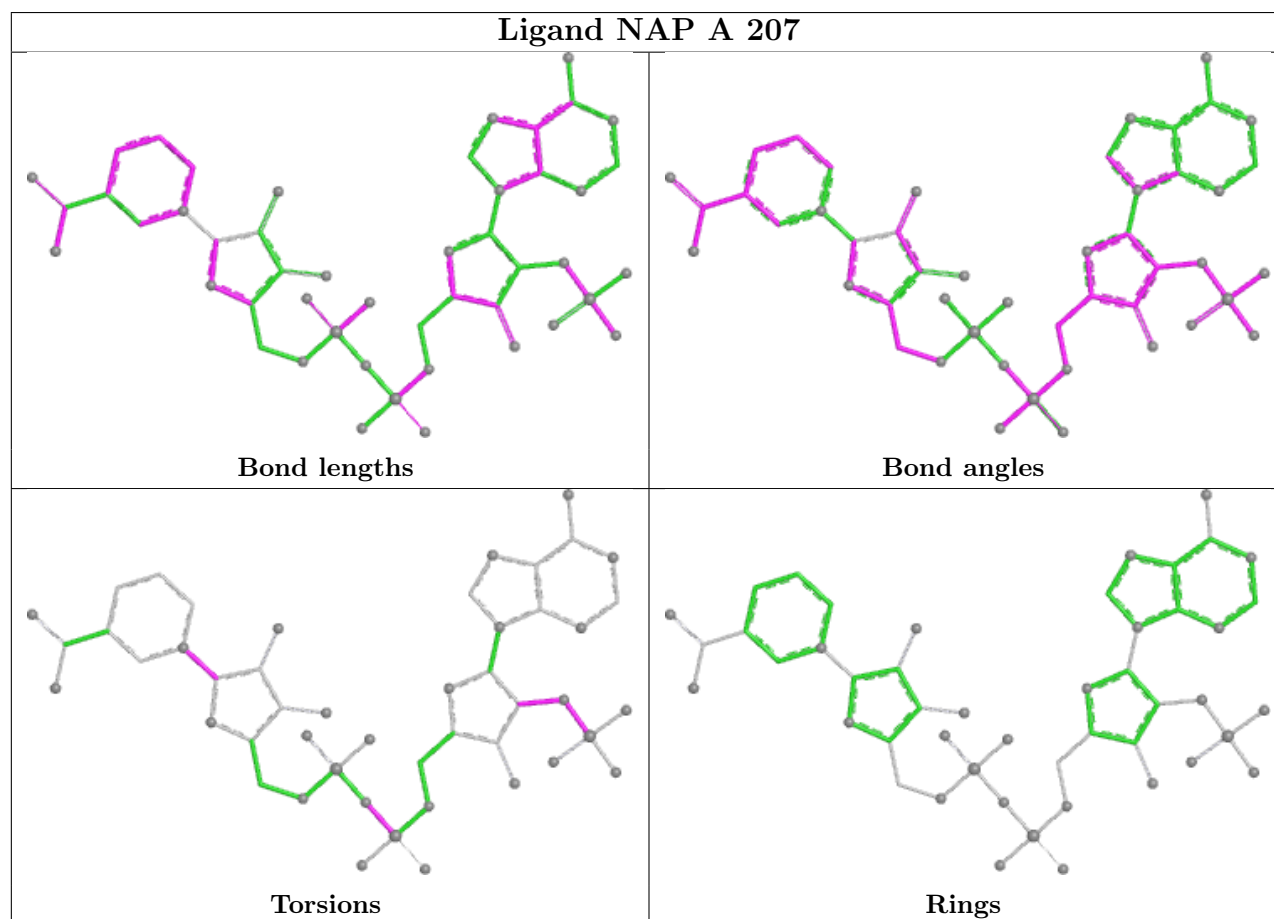
There are no ring outliers.

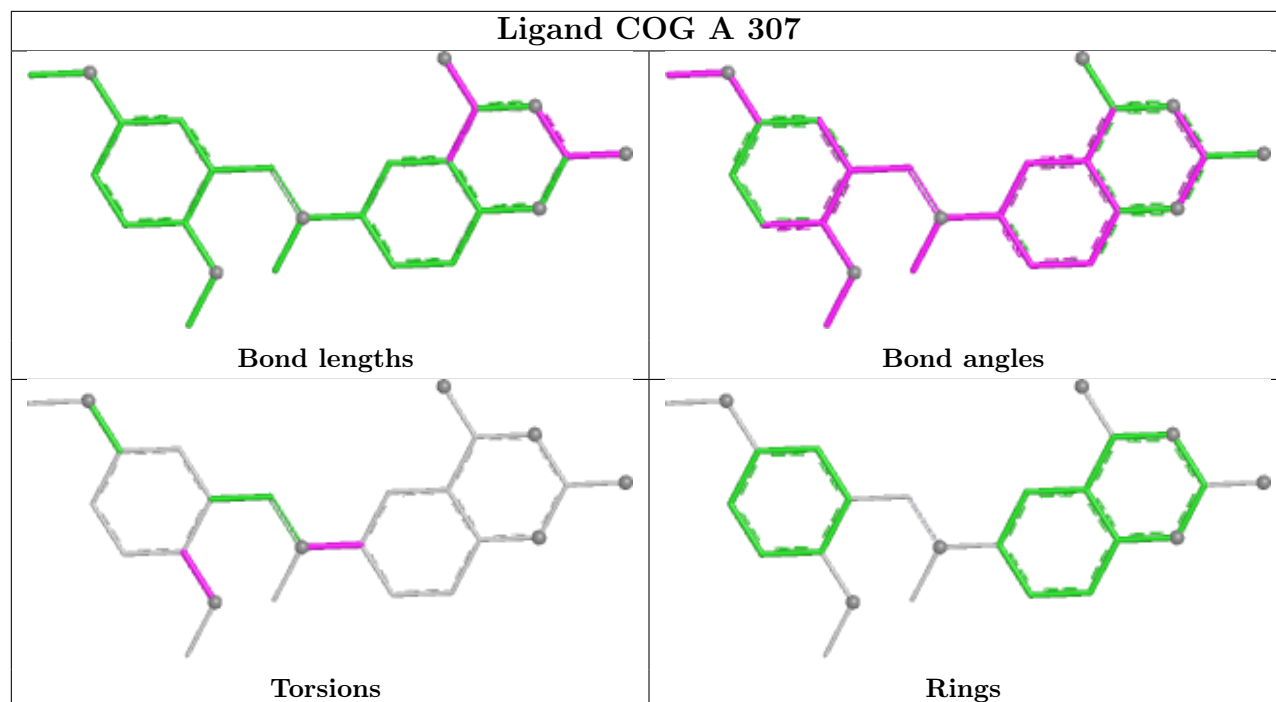
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	207	NAP	4	0
3	A	307	COG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	87:ASP	C	88:LEU	N	1.17

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	206/206 (100%)	-0.10	9 (4%)	39 41	10, 22, 45, 48	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	LEU	4.7
1	A	2	ASN	3.7
1	A	86	LEU	3.5
1	A	87	ASP	3.3
1	A	1	MET	3.2
1	A	49	PHE	3.1
1	A	85	SER	2.3
1	A	83	ASN	2.2
1	A	90	ASN	2.1

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](#)

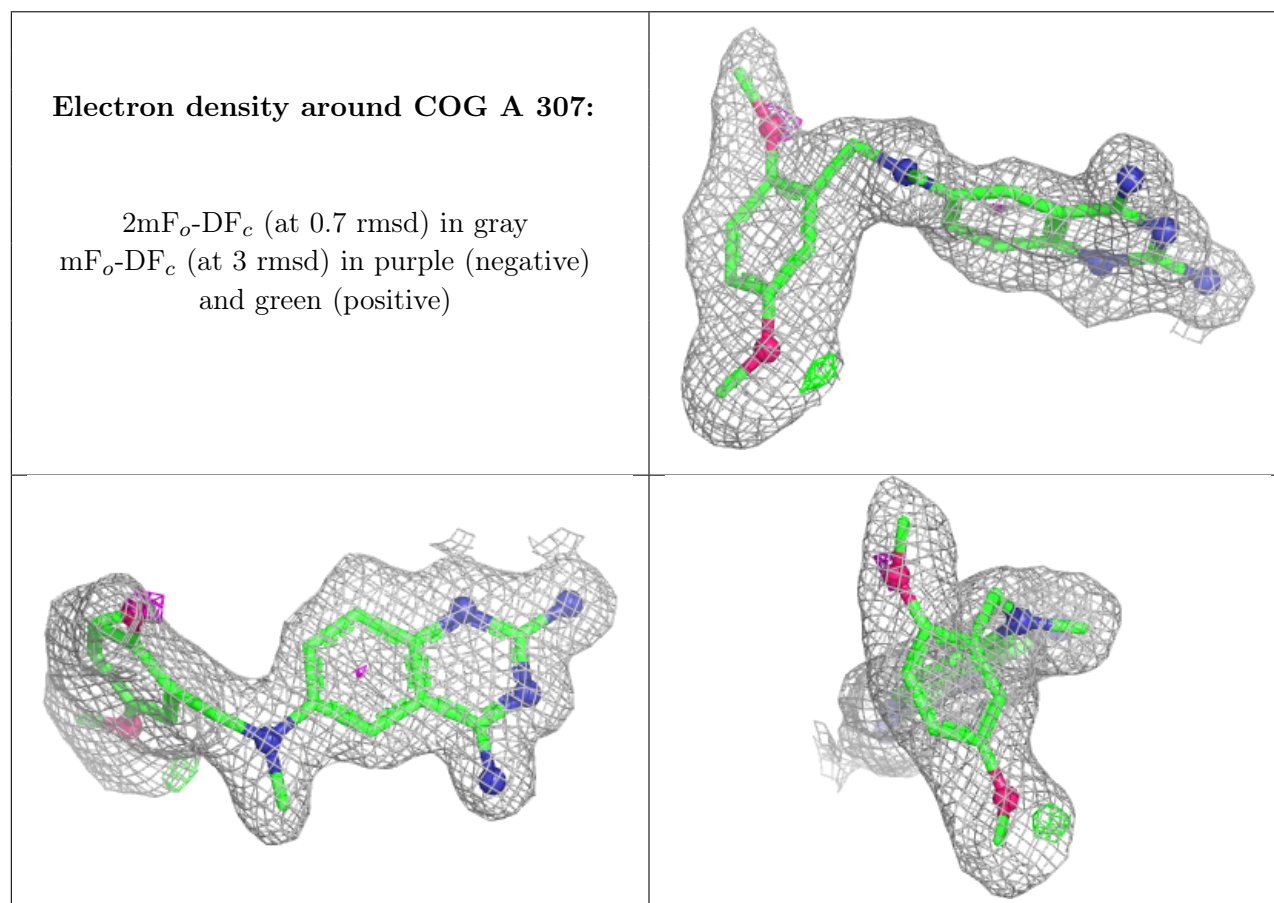
There are no oligosaccharides in this entry.

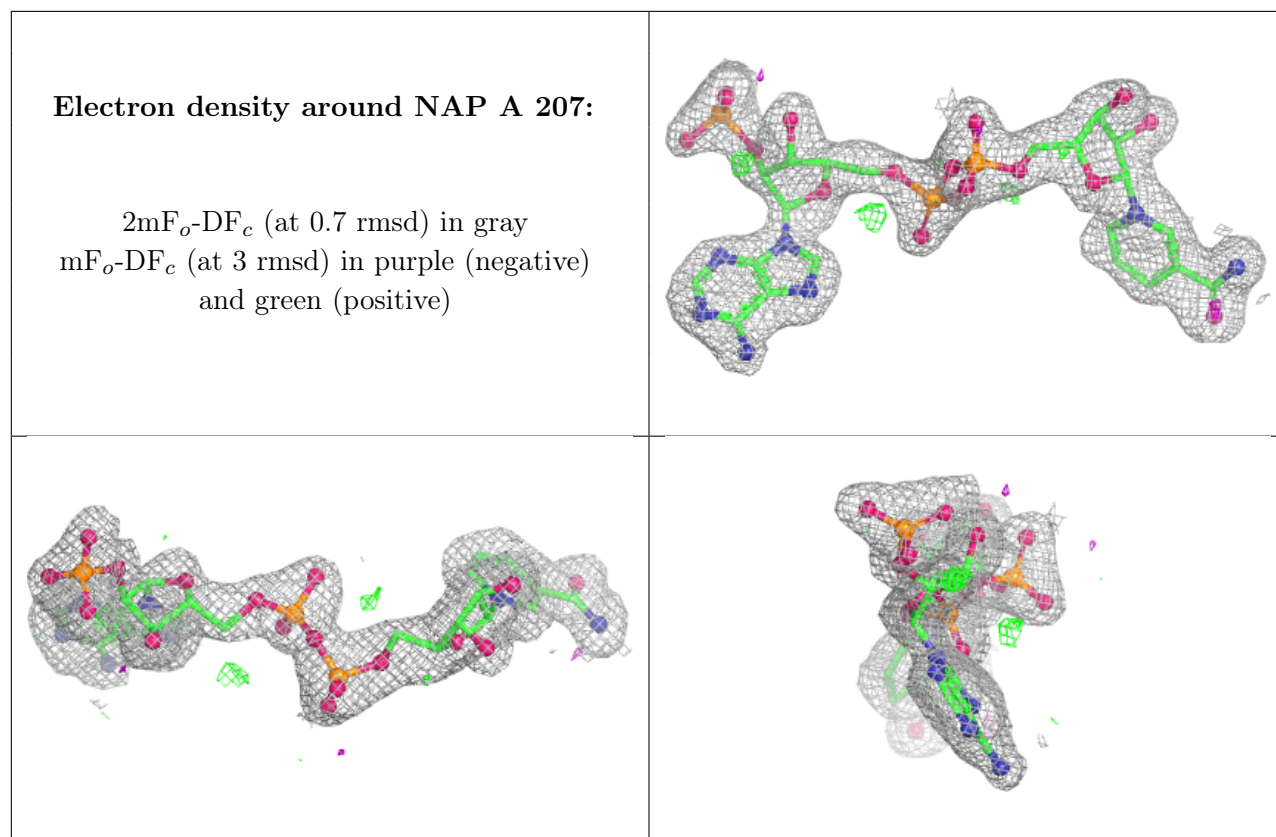
6.4 Ligands [i](#)

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
3	COG	A	307	25/25	0.89	0.07	8,23,36,37	0
2	NAP	A	207	48/48	0.94	0.06	12,25,31,33	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.