



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 11:23 PM EDT

PDB ID : 1LY4
Title : Analysis of quinazoline and PYRIDO[2,3D]PYRIMIDINE N9-C10 reversed bridge antifolates in complex with NADP⁺ and *Pneumocystis carinii* dihydrofolate reductase
Authors : Cody, V.; Galitsky, N.; Luft, J.R.; Pangborn, W.; Queener, S.F.; Gangjee, A.
Deposited on : 2002-06-06
Resolution : 2.10 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

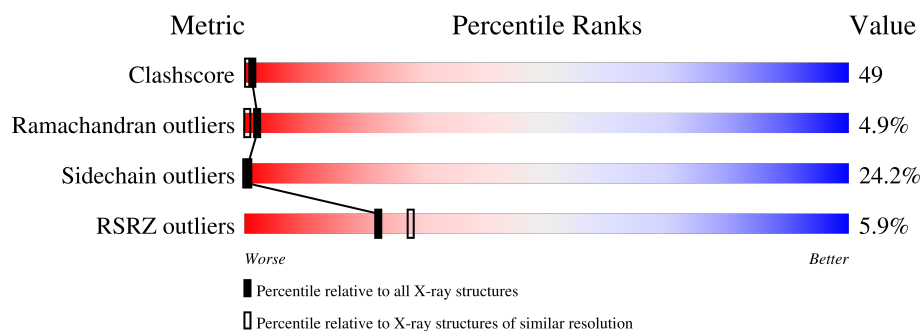
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 1784 atoms, of which 0 are hydrogens and 0 are deuteriums.

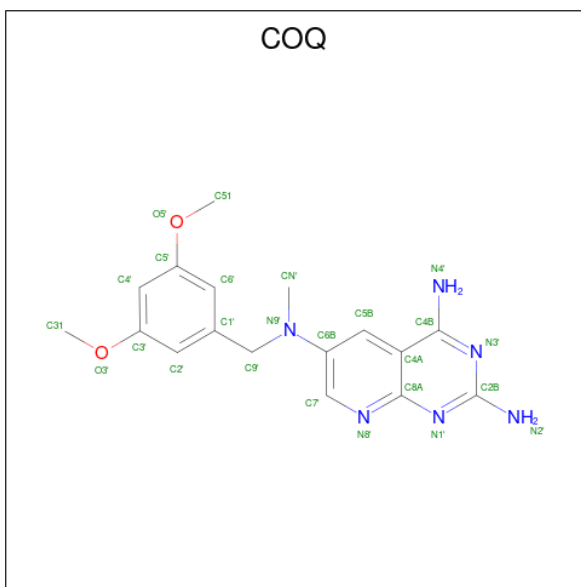
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	205	1678	1081	287	304	6	0	0	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	17	6	2		

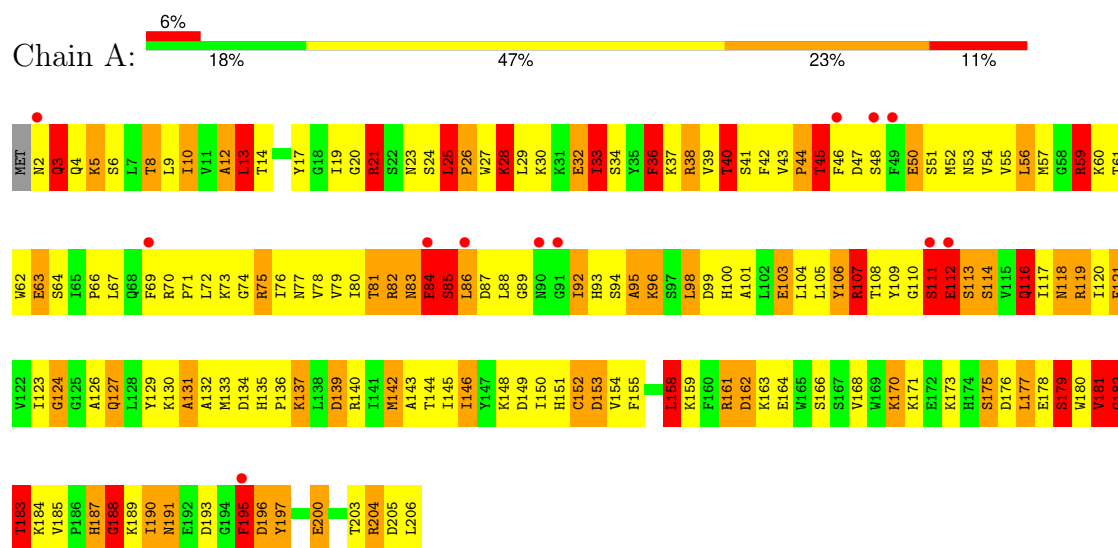
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		

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	37.05Å 43.13Å 60.73Å 90.00° 94.60° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10 30.46 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.10) 90.0 (30.46-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.10Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.193 , (Not available) 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 97.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1784	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.81% 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: NAP, COQ

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	1.16	0/1720	2.90	143/2320 (6.2%)

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

There are no bond length outliers.

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	ASP	CB-CG-OD1	23.92	139.83	118.30
1	A	140	ARG	NE-CZ-NH1	23.76	132.18	120.30
1	A	204	ARG	CD-NE-CZ	22.01	154.41	123.60
1	A	59	ARG	NE-CZ-NH2	-18.60	111.00	120.30
1	A	107	ARG	NE-CZ-NH2	-17.21	111.69	120.30
1	A	140	ARG	NE-CZ-NH2	-16.17	112.22	120.30
1	A	38	ARG	NE-CZ-NH1	16.00	128.30	120.30
1	A	203	THR	CA-CB-CG2	15.73	134.43	112.40
1	A	75	ARG	NE-CZ-NH2	-15.14	112.73	120.30
1	A	59	ARG	NE-CZ-NH1	14.12	127.36	120.30
1	A	21	ARG	NE-CZ-NH1	-12.51	114.05	120.30
1	A	176	ASP	CB-CA-C	12.36	135.12	110.40
1	A	196	ASP	CB-CG-OD1	11.39	128.55	118.30
1	A	87	ASP	CB-CG-OD1	11.34	128.50	118.30
1	A	176	ASP	CA-CB-CG	11.17	137.97	113.40
1	A	52	MET	CA-CB-CG	10.51	131.17	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ARG	CD-NE-CZ	-10.39	109.05	123.60
1	A	139	ASP	CB-CG-OD1	10.08	127.37	118.30
1	A	200	GLU	CG-CD-OE1	10.03	138.36	118.30
1	A	162	ASP	OD1-CG-OD2	-9.87	104.54	123.30
1	A	21	ARG	NH1-CZ-NH2	9.81	130.19	119.40
1	A	75	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	A	168	VAL	CA-CB-CG2	9.58	125.27	110.90
1	A	27	TRP	C-N-CA	9.57	145.62	121.70
1	A	148	LYS	CA-CB-CG	9.45	134.19	113.40
1	A	162	ASP	CA-CB-CG	9.34	133.94	113.40
1	A	95	ALA	CB-CA-C	9.31	124.06	110.10
1	A	21	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	A	38	ARG	NH1-CZ-NH2	-8.96	109.54	119.40
1	A	96	LYS	CA-CB-CG	8.96	133.11	113.40
1	A	188	GLY	CA-C-O	8.86	136.55	120.60
1	A	63	GLU	OE1-CD-OE2	-8.62	112.95	123.30
1	A	107	ARG	NH1-CZ-NH2	8.56	128.81	119.40
1	A	184	LYS	CB-CA-C	8.39	127.17	110.40
1	A	178	GLU	OE1-CD-OE2	-8.33	113.31	123.30
1	A	205	ASP	CB-CG-OD1	8.23	125.71	118.30
1	A	153	ASP	CB-CG-OD1	8.15	125.63	118.30
1	A	189	LYS	CB-CA-C	8.07	126.53	110.40
1	A	200	GLU	OE1-CD-OE2	-7.96	113.75	123.30
1	A	100	HIS	O-C-N	7.95	135.42	122.70
1	A	99	ASP	CB-CG-OD1	-7.85	111.23	118.30
1	A	134	ASP	CB-CG-OD2	7.79	125.31	118.30
1	A	13	LEU	CB-CG-CD2	7.72	124.12	111.00
1	A	178	GLU	CG-CD-OE1	7.63	133.56	118.30
1	A	38	ARG	N-CA-CB	7.55	124.19	110.60
1	A	204	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	52	MET	CB-CA-C	7.50	125.40	110.40
1	A	164	GLU	CG-CD-OE2	-7.31	103.68	118.30
1	A	183	THR	CA-C-O	7.30	135.42	120.10
1	A	96	LYS	CB-CA-C	7.22	124.83	110.40
1	A	119	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	9	LEU	CB-CG-CD2	-7.20	98.76	111.00
1	A	164	GLU	CG-CD-OE1	7.03	132.36	118.30
1	A	9	LEU	CA-C-O	-6.94	105.53	120.10
1	A	161	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	96	LYS	N-CA-CB	-6.89	98.19	110.60
1	A	32	GLU	CG-CD-OE1	6.83	131.96	118.30
1	A	205	ASP	O-C-N	6.83	133.62	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	SER	O-C-N	6.81	133.59	122.70
1	A	124	GLY	C-N-CA	6.76	136.51	122.30
1	A	103	GLU	OE1-CD-OE2	-6.71	115.25	123.30
1	A	112	GLU	CB-CG-CD	6.70	132.29	114.20
1	A	184	LYS	N-CA-CB	-6.69	98.55	110.60
1	A	100	HIS	CA-CB-CG	-6.60	102.38	113.60
1	A	161	ARG	NE-CZ-NH2	6.49	123.54	120.30
1	A	82	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	A	132	ALA	O-C-N	-6.44	112.40	122.70
1	A	195	PHE	CA-CB-CG	6.44	129.35	113.90
1	A	119	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	A	100	HIS	N-CA-CB	6.38	122.09	110.60
1	A	55	VAL	CA-CB-CG2	-6.33	101.40	110.90
1	A	106	TYR	CB-CG-CD2	6.30	124.78	121.00
1	A	13	LEU	CA-CB-CG	6.29	129.76	115.30
1	A	127	GLN	O-C-N	6.27	132.74	122.70
1	A	75	ARG	CD-NE-CZ	6.24	132.33	123.60
1	A	184	LYS	CA-CB-CG	-6.23	99.69	113.40
1	A	152	CYS	O-C-N	6.14	132.53	122.70
1	A	59	ARG	CA-CB-CG	6.12	126.87	113.40
1	A	36	PHE	CB-CA-C	6.12	122.64	110.40
1	A	106	TYR	CB-CG-CD1	-6.11	117.33	121.00
1	A	161	ARG	NH1-CZ-NH2	-6.11	112.68	119.40
1	A	2	ASN	CA-CB-CG	6.08	126.78	113.40
1	A	103	GLU	CA-C-O	-6.04	107.42	120.10
1	A	134	ASP	CA-CB-CG	6.03	126.67	113.40
1	A	98	LEU	CB-CG-CD2	-6.03	100.75	111.00
1	A	3	GLN	CA-C-N	-6.02	103.96	117.20
1	A	12	ALA	N-CA-CB	5.98	118.47	110.10
1	A	181	VAL	CB-CA-C	5.98	122.76	111.40
1	A	113	SER	C-N-CA	5.96	136.59	121.70
1	A	8	THR	N-CA-CB	5.94	121.59	110.30
1	A	149	ASP	CA-CB-CG	-5.94	100.34	113.40
1	A	73	LYS	CA-C-N	-5.93	104.34	116.20
1	A	116	GLN	CB-CG-CD	5.86	126.84	111.60
1	A	92	ILE	CB-CG1-CD1	5.80	130.14	113.90
1	A	134	ASP	OD1-CG-OD2	-5.80	112.28	123.30
1	A	161	ARG	C-N-CA	5.78	136.14	121.70
1	A	131	ALA	CA-C-N	5.64	129.60	117.20
1	A	119	ARG	CD-NE-CZ	-5.62	115.73	123.60
1	A	26	PRO	N-CA-C	5.60	126.65	112.10
1	A	182	GLY	N-CA-C	-5.58	99.15	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	VAL	CA-CB-CG1	5.55	119.23	110.90
1	A	73	LYS	CA-C-O	5.55	131.76	120.10
1	A	103	GLU	N-CA-CB	5.55	120.58	110.60
1	A	111	SER	C-N-CA	5.53	135.52	121.70
1	A	158	LEU	CB-CG-CD1	-5.51	101.63	111.00
1	A	33	ILE	CB-CA-C	5.47	122.55	111.60
1	A	40	THR	CA-CB-CG2	5.46	120.04	112.40
1	A	118	ASN	C-N-CA	5.46	135.34	121.70
1	A	146	ILE	C-N-CA	5.44	135.30	121.70
1	A	190	ILE	O-C-N	5.43	131.38	122.70
1	A	8	THR	C-N-CA	5.42	135.24	121.70
1	A	155	PHE	N-CA-CB	-5.38	100.91	110.60
1	A	143	ALA	CB-CA-C	-5.37	102.05	110.10
1	A	129	TYR	CB-CG-CD2	5.32	124.19	121.00
1	A	63	GLU	CB-CG-CD	5.31	128.54	114.20
1	A	142	MET	CA-CB-CG	5.31	122.33	113.30
1	A	204	ARG	CA-CB-CG	5.27	124.99	113.40
1	A	203	THR	CA-CB-OG1	-5.24	97.99	109.00
1	A	47	ASP	O-C-N	5.24	131.09	122.70
1	A	78	VAL	CA-C-O	-5.24	109.09	120.10
1	A	185	VAL	CA-CB-CG2	5.22	118.73	110.90
1	A	187	HIS	CA-C-N	5.21	126.63	116.20
1	A	200	GLU	CG-CD-OE2	-5.21	107.88	118.30
1	A	114	SER	N-CA-CB	-5.17	102.74	110.50
1	A	132	ALA	CA-C-O	5.14	130.90	120.10
1	A	179	SER	CA-C-O	-5.14	109.30	120.10
1	A	25	LEU	CA-CB-CG	-5.14	103.48	115.30
1	A	28	LYS	CA-CB-CG	5.13	124.68	113.40
1	A	158	LEU	CA-C-O	-5.12	109.35	120.10
1	A	81	THR	C-N-CA	5.12	134.49	121.70
1	A	28	LYS	N-CA-CB	-5.10	101.42	110.60
1	A	181	VAL	CA-C-N	5.09	126.38	116.20
1	A	107	ARG	CD-NE-CZ	5.09	130.72	123.60
1	A	121	PHE	CZ-CE2-CD2	-5.08	114.00	120.10
1	A	118	ASN	N-CA-CB	-5.07	101.47	110.60
1	A	113	SER	CA-C-O	5.06	130.72	120.10
1	A	162	ASP	N-CA-CB	5.05	119.69	110.60
1	A	197	TYR	CG-CD2-CE2	5.04	125.33	121.30
1	A	175	SER	C-N-CA	-5.04	109.10	121.70
1	A	161	ARG	CG-CD-NE	-5.03	101.23	111.80
1	A	10	ILE	CB-CA-C	5.02	121.64	111.60
1	A	105	LEU	CB-CG-CD2	-5.02	102.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	177	LEU	CB-CG-CD2	5.01	119.52	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1678	0	1680	172	0
2	A	48	0	25	10	0
3	A	25	0	20	3	0
4	A	33	0	0	15	0
All	All	1784	0	1725	172	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 49.

All (172) 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:40:THR:CG2	1:A:75:ARG:HH11	1.60	1.13
1:A:104:LEU:HD23	1:A:104:LEU:O	1.55	1.06
1:A:25:LEU:HD22	3:A:307:COQ:HCN2	1.14	1.06
1:A:40:THR:HG22	1:A:75:ARG:HH11	1.16	1.05
1:A:187:HIS:CD2	1:A:188:GLY:H	1.73	1.05
1:A:81:THR:O	1:A:81:THR:HG23	1.68	0.93
1:A:98:LEU:HD12	1:A:98:LEU:H	1.33	0.91
1:A:43:VAL:C	4:A:215:HOH:O	2.09	0.91
1:A:162:ASP:HB2	4:A:234:HOH:O	1.70	0.90
1:A:187:HIS:HD2	1:A:188:GLY:N	1.67	0.90
1:A:38:ARG:HD3	1:A:183:THR:HG21	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASN:HB2	1:A:92:ILE:HD12	1.53	0.89
1:A:5:LYS:HE2	1:A:118:ASN:O	1.74	0.87
1:A:135:HIS:HD2	1:A:137:LYS:H	1.23	0.85
1:A:50:GLU:HG2	1:A:51:SER:N	1.90	0.84
1:A:40:THR:HG22	1:A:75:ARG:NH1	1.95	0.81
1:A:50:GLU:OE2	1:A:116:GLN:HB2	1.81	0.81
1:A:135:HIS:CD2	1:A:137:LYS:H	2.00	0.79
1:A:187:HIS:HD2	1:A:188:GLY:H	0.84	0.78
1:A:3:GLN:HA	1:A:106:TYR:HE2	1.48	0.78
1:A:3:GLN:HG3	1:A:137:LYS:HG2	1.65	0.78
1:A:40:THR:CG2	1:A:75:ARG:NH1	2.44	0.78
1:A:59:ARG:O	1:A:62:TRP:HB3	1.85	0.77
1:A:83:ASN:O	1:A:85:SER:N	2.19	0.76
1:A:36:PHE:O	1:A:40:THR:HB	1.86	0.75
1:A:25:LEU:H	1:A:25:LEU:HD23	1.51	0.75
1:A:50:GLU:OE1	4:A:238:HOH:O	2.06	0.74
1:A:86:LEU:H	1:A:86:LEU:HD12	1.52	0.74
1:A:104:LEU:HD23	1:A:104:LEU:C	2.07	0.74
1:A:50:GLU:CD	1:A:116:GLN:HG3	2.08	0.74
1:A:150:ILE:CD1	1:A:195:PHE:HE2	1.99	0.74
1:A:107:ARG:HH11	1:A:107:ARG:HG2	1.52	0.73
1:A:59:ARG:NH2	2:A:207:NAP:O2X	2.22	0.72
1:A:50:GLU:HG3	1:A:116:GLN:HG2	1.71	0.72
1:A:20:GLY:O	1:A:152:CYS:HB3	1.88	0.71
1:A:187:HIS:CD2	1:A:188:GLY:N	2.50	0.71
1:A:66:PRO:CG	1:A:69:PHE:HD1	2.05	0.69
1:A:139:ASP:HB3	1:A:206:LEU:HD11	1.73	0.69
1:A:25:LEU:CD2	3:A:307:COQ:HCN2	2.09	0.68
1:A:98:LEU:CD1	4:A:231:HOH:O	2.41	0.68
1:A:77:ASN:HB2	1:A:92:ILE:CD1	2.24	0.68
1:A:135:HIS:CD2	1:A:137:LYS:HB2	2.30	0.67
1:A:60:LYS:O	1:A:63:GLU:HB2	1.94	0.67
1:A:150:ILE:CD1	1:A:195:PHE:CE2	2.77	0.67
1:A:50:GLU:HG3	1:A:116:GLN:CG	2.25	0.66
1:A:135:HIS:HD2	1:A:137:LYS:N	1.92	0.66
1:A:38:ARG:HD3	1:A:183:THR:CG2	2.25	0.66
1:A:170:LYS:HG3	4:A:229:HOH:O	1.94	0.65
1:A:150:ILE:HD13	1:A:195:PHE:HE2	1.63	0.64
1:A:42:PHE:CD2	1:A:42:PHE:O	2.51	0.64
1:A:79:VAL:O	1:A:94:SER:HA	1.98	0.63
1:A:81:THR:O	1:A:81:THR:CG2	2.41	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:CE	1:A:118:ASN:O	2.46	0.63
1:A:45:THR:O	1:A:48:SER:OG	2.15	0.63
1:A:126:ALA:HB2	1:A:154:VAL:CG1	2.27	0.63
1:A:66:PRO:HG2	1:A:69:PHE:HB2	1.82	0.62
1:A:171:LYS:HE2	1:A:200:GLU:OE2	2.00	0.62
1:A:50:GLU:OE2	1:A:116:GLN:CB	2.47	0.62
1:A:104:LEU:O	1:A:108:THR:OG1	2.08	0.62
1:A:182:GLY:O	1:A:183:THR:C	2.38	0.61
1:A:150:ILE:HD11	1:A:195:PHE:CE2	2.35	0.61
1:A:25:LEU:H	1:A:25:LEU:CD2	2.07	0.61
1:A:170:LYS:CG	4:A:229:HOH:O	2.47	0.61
1:A:66:PRO:CB	1:A:69:PHE:HD1	2.14	0.61
1:A:80:ILE:O	2:A:207:NAP:H1B	2.00	0.61
1:A:19:ILE:O	2:A:207:NAP:H2N	2.00	0.60
1:A:43:VAL:HG12	1:A:118:ASN:OD1	2.02	0.60
1:A:193:ASP:N	4:A:227:HOH:O	2.33	0.60
1:A:3:GLN:HA	1:A:106:TYR:CE2	2.35	0.59
1:A:98:LEU:HD12	4:A:231:HOH:O	2.00	0.59
1:A:38:ARG:NE	1:A:183:THR:OG1	2.35	0.59
1:A:44:PRO:N	4:A:215:HOH:O	2.27	0.59
1:A:126:ALA:HB3	2:A:207:NAP:O1N	2.01	0.59
1:A:21:ARG:HD2	1:A:151:HIS:O	2.03	0.59
1:A:109:TYR:O	1:A:111:SER:N	2.33	0.59
1:A:40:THR:HG23	1:A:75:ARG:CD	2.33	0.59
1:A:107:ARG:HG2	1:A:107:ARG:NH1	2.16	0.58
1:A:25:LEU:HD23	1:A:25:LEU:N	2.17	0.58
1:A:50:GLU:OE2	1:A:116:GLN:HG3	2.04	0.57
1:A:74:GLY:O	1:A:75:ARG:HG3	2.04	0.57
1:A:59:ARG:NH2	2:A:207:NAP:P2B	2.78	0.57
1:A:42:PHE:CE2	1:A:181:VAL:O	2.58	0.56
1:A:45:THR:HG22	1:A:46:PHE:N	2.20	0.56
1:A:77:ASN:CB	1:A:92:ILE:HD12	2.29	0.56
1:A:106:TYR:CD1	1:A:106:TYR:N	2.72	0.56
1:A:95:ALA:HB3	1:A:101:ALA:HB2	1.88	0.55
1:A:126:ALA:HB2	1:A:154:VAL:HG11	1.87	0.55
1:A:98:LEU:HD11	1:A:131:ALA:HB1	1.90	0.54
1:A:40:THR:HG23	1:A:75:ARG:HD3	1.89	0.54
1:A:188:GLY:O	1:A:190:ILE:HD12	2.07	0.54
1:A:42:PHE:CE2	4:A:215:HOH:O	2.59	0.54
1:A:66:PRO:HB2	1:A:69:PHE:HD1	1.71	0.54
1:A:191:ASN:HA	1:A:195:PHE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:C	1:A:104:LEU:CD2	2.75	0.54
1:A:38:ARG:CD	1:A:183:THR:CG2	2.86	0.53
1:A:5:LYS:HD2	1:A:120:ILE:HG13	1.89	0.53
1:A:86:LEU:HD12	1:A:86:LEU:N	2.18	0.53
1:A:88:LEU:HD13	1:A:89:GLY:N	2.23	0.53
1:A:163:LYS:O	1:A:166:SER:OG	2.27	0.53
1:A:98:LEU:H	1:A:98:LEU:CD1	2.14	0.52
1:A:80:ILE:N	1:A:80:ILE:HD12	2.24	0.51
1:A:59:ARG:HH22	2:A:207:NAP:P2B	2.33	0.51
1:A:12:ALA:O	2:A:207:NAP:N7N	2.43	0.51
1:A:28:LYS:O	1:A:29:LEU:HD12	2.11	0.51
1:A:66:PRO:CG	1:A:69:PHE:CD1	2.91	0.51
1:A:106:TYR:N	1:A:106:TYR:HD1	2.09	0.51
1:A:150:ILE:HD11	1:A:195:PHE:CD2	2.46	0.51
1:A:182:GLY:O	1:A:183:THR:O	2.30	0.50
1:A:119:ARG:NH2	1:A:180:TRP:O	2.40	0.49
1:A:38:ARG:CD	1:A:183:THR:HG21	2.34	0.49
1:A:8:THR:CG2	1:A:142:MET:HG2	2.43	0.49
1:A:32:GLU:HG2	1:A:144:THR:HG21	1.95	0.49
1:A:66:PRO:HB2	1:A:69:PHE:CD1	2.48	0.49
1:A:159:LYS:HE2	1:A:162:ASP:OD2	2.12	0.49
1:A:38:ARG:CD	1:A:183:THR:OG1	2.61	0.48
1:A:56:LEU:N	1:A:121:PHE:O	2.45	0.48
1:A:29:LEU:O	1:A:33:ILE:HB	2.13	0.48
1:A:150:ILE:HD13	1:A:195:PHE:CE2	2.47	0.48
1:A:42:PHE:CE1	4:A:215:HOH:O	2.67	0.48
1:A:111:SER:HB2	1:A:112:GLU:OE2	2.13	0.48
1:A:70:ARG:HA	1:A:71:PRO:C	2.34	0.48
1:A:14:THR:HA	1:A:146:ILE:O	2.14	0.47
1:A:42:PHE:CD2	4:A:215:HOH:O	2.67	0.47
1:A:130:LYS:O	1:A:130:LYS:HG3	2.00	0.47
1:A:175:SER:O	1:A:179:SER:HB3	2.15	0.47
1:A:10:ILE:HD12	1:A:39:VAL:HG11	1.96	0.47
1:A:86:LEU:HD12	1:A:86:LEU:C	2.34	0.46
1:A:181:VAL:CG2	1:A:182:GLY:H	2.27	0.46
1:A:161:ARG:NH2	1:A:200:GLU:OE1	2.41	0.46
1:A:161:ARG:HH21	1:A:200:GLU:CD	2.19	0.46
1:A:86:LEU:C	1:A:86:LEU:CD1	2.84	0.45
1:A:25:LEU:O	1:A:25:LEU:HG	2.15	0.45
1:A:135:HIS:HA	1:A:136:PRO:HD2	1.82	0.45
1:A:54:VAL:HG22	1:A:76:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:HB3	1:A:104:LEU:HD11	1.98	0.45
1:A:61:THR:O	1:A:62:TRP:C	2.54	0.44
1:A:57:MET:HA	1:A:124:GLY:O	2.17	0.44
1:A:126:ALA:HB2	1:A:154:VAL:HG12	1.99	0.44
1:A:17:TYR:CE1	1:A:159:LYS:HA	2.52	0.44
1:A:25:LEU:HD22	3:A:307:COQ:CN'	2.09	0.44
1:A:145:ILE:HD12	1:A:161:ARG:NE	2.32	0.44
1:A:42:PHE:CD1	4:A:215:HOH:O	2.69	0.44
1:A:13:LEU:HD11	1:A:145:ILE:HD13	2.00	0.44
1:A:23:ASN:O	1:A:64:SER:HB2	2.17	0.44
1:A:66:PRO:HG2	1:A:69:PHE:CD1	2.53	0.43
1:A:43:VAL:CA	4:A:215:HOH:O	2.61	0.43
1:A:30:LYS:HB3	1:A:30:LYS:HE2	1.85	0.43
1:A:135:HIS:CD2	1:A:137:LYS:N	2.76	0.43
1:A:127:GLN:HB3	2:A:207:NAP:C8A	2.48	0.43
1:A:50:GLU:OE2	1:A:116:GLN:CG	2.66	0.43
1:A:88:LEU:HD22	1:A:88:LEU:HA	1.87	0.43
1:A:159:LYS:HB3	1:A:159:LYS:HE3	1.68	0.43
1:A:74:GLY:C	1:A:75:ARG:HG3	2.39	0.43
1:A:126:ALA:CB	1:A:154:VAL:CG1	2.97	0.43
1:A:13:LEU:CD1	1:A:145:ILE:HD13	2.48	0.43
1:A:32:GLU:CG	1:A:144:THR:HG21	2.49	0.42
1:A:145:ILE:O	1:A:197:TYR:HA	2.20	0.42
1:A:59:ARG:O	1:A:62:TRP:N	2.53	0.42
1:A:41:SER:HA	1:A:53:ASN:HD22	1.85	0.42
1:A:59:ARG:O	1:A:62:TRP:CB	2.62	0.42
1:A:123:ILE:HG21	1:A:123:ILE:HD13	1.86	0.42
1:A:59:ARG:HG2	2:A:207:NAP:O2X	2.19	0.42
1:A:23:ASN:O	1:A:23:ASN:CG	2.58	0.41
1:A:72:LEU:O	1:A:77:ASN:ND2	2.52	0.41
1:A:133:MET:CE	1:A:158:LEU:HD22	2.50	0.41
1:A:66:PRO:O	1:A:70:ARG:HG2	2.20	0.41
1:A:80:ILE:N	1:A:80:ILE:CD1	2.83	0.41
1:A:50:GLU:CG	1:A:116:GLN:CG	2.96	0.41
1:A:83:ASN:O	1:A:84:GLU:C	2.57	0.40
1:A:42:PHE:CG	4:A:215:HOH:O	2.75	0.40
1:A:80:ILE:HG22	2:A:207:NAP:N3A	2.37	0.40
1:A:42:PHE:O	1:A:42:PHE:CG	2.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	203/206 (98%)	169 (83%)	24 (12%)	10 (5%)	2 0

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	PRO
1	A	111	SER
1	A	183	THR
1	A	188	GLY
1	A	84	GLU
1	A	110	GLY
1	A	181	VAL
1	A	45	THR
1	A	85	SER
1	A	182	GLY

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	186/187 (100%)	141 (76%)	45 (24%)	0 0

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN

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Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	LYS
1	A	13	LEU
1	A	21	ARG
1	A	24	SER
1	A	25	LEU
1	A	28	LYS
1	A	33	ILE
1	A	34	SER
1	A	36	PHE
1	A	37	LYS
1	A	40	THR
1	A	44	PRO
1	A	45	THR
1	A	50	GLU
1	A	56	LEU
1	A	59	ARG
1	A	67	LEU
1	A	82	ARG
1	A	83	ASN
1	A	84	GLU
1	A	85	SER
1	A	86	LEU
1	A	96	LYS
1	A	103	GLU
1	A	107	ARG
1	A	111	SER
1	A	112	GLU
1	A	113	SER
1	A	114	SER
1	A	116	GLN
1	A	117	ILE
1	A	137	LYS
1	A	153	ASP
1	A	158	LEU
1	A	170	LYS
1	A	173	LYS
1	A	177	LEU
1	A	179	SER
1	A	181	VAL
1	A	183	THR
1	A	191	ASN

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Mol	Chain	Res	Type
1	A	195	PHE
1	A	196	ASP

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

Mol	Chain	Res	Type
1	A	4	GLN
1	A	116	GLN
1	A	127	GLN
1	A	135	HIS
1	A	174	HIS
1	A	187	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 monosaccharides 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	$\# Z > 2$
3	COQ	A	307	-	27,27,27	1.57	4 (14%)	36,38,38	3.08	15 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	A	207	-	46,52,52	3.46	21 (45%)	61,80,80	3.21	27 (44%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COQ	A	307	-	-	6/12/12/12	0/3/3/3
2	NAP	A	207	-	-	3/31/67/67	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	207	NAP	C4N-C3N	11.07	1.56	1.39
2	A	207	NAP	O4B-C4B	-8.70	1.25	1.45
2	A	207	NAP	P2B-O2B	8.10	1.73	1.59
2	A	207	NAP	C2N-N1N	7.33	1.43	1.35
2	A	207	NAP	C5N-C4N	6.12	1.49	1.38
2	A	207	NAP	O4D-C1D	6.07	1.48	1.40
2	A	207	NAP	C3B-C4B	4.95	1.65	1.53
3	A	307	COQ	C7'-N8'	4.63	1.39	1.31
2	A	207	NAP	C2N-C3N	-3.81	1.33	1.39
3	A	307	COQ	C4B-C4A	-3.72	1.41	1.45
2	A	207	NAP	O3B-C3B	3.63	1.51	1.43
2	A	207	NAP	C6A-C5A	3.34	1.55	1.43
2	A	207	NAP	PA-O5B	3.30	1.72	1.59
2	A	207	NAP	O3D-C3D	3.00	1.50	1.43
2	A	207	NAP	O4D-C4D	2.91	1.51	1.45
2	A	207	NAP	C6N-N1N	2.70	1.41	1.35
2	A	207	NAP	PA-O2A	-2.56	1.43	1.55
2	A	207	NAP	PN-O1N	-2.41	1.42	1.50
2	A	207	NAP	O2D-C2D	-2.38	1.37	1.43
2	A	207	NAP	C6N-C5N	-2.16	1.34	1.38
3	A	307	COQ	C6'-C1'	2.10	1.42	1.39
3	A	307	COQ	O5'-C5'	2.08	1.41	1.37
2	A	207	NAP	O4B-C1B	2.05	1.43	1.40
2	A	207	NAP	C5A-N7A	2.05	1.47	1.39
2	A	207	NAP	C3D-C4D	2.02	1.58	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	207	NAP	C5N-C4N-C3N	-9.19	111.33	120.36
2	A	207	NAP	O4B-C1B-N9A	8.20	119.62	108.75
3	A	307	COQ	N1'-C2B-N3'	-7.78	117.32	127.21
2	A	207	NAP	C4B-O4B-C1B	7.12	116.44	109.92
2	A	207	NAP	C4D-O4D-C1D	-7.04	103.47	109.92
3	A	307	COQ	N2'-C2B-N1'	6.91	128.57	117.79
2	A	207	NAP	C2N-C3N-C4N	6.24	125.52	118.26
3	A	307	COQ	C9'-N9'-C6B	-5.99	112.91	120.17
2	A	207	NAP	O7N-C7N-C3N	-5.83	112.46	119.60
2	A	207	NAP	O3B-C3B-C4B	-5.49	95.30	111.08
3	A	307	COQ	C51-O5'-C5'	-5.28	106.18	117.50
3	A	307	COQ	C4A-C4B-N4'	5.24	129.49	121.45
3	A	307	COQ	C2B-N1'-C8A	5.09	120.97	115.48
2	A	207	NAP	P2B-O2B-C2B	4.84	136.35	123.43
3	A	307	COQ	CN'-N9'-C6B	4.80	127.55	119.59
3	A	307	COQ	C4A-C4B-N3'	-4.60	117.03	121.97
2	A	207	NAP	O3-PA-O1A	-4.41	97.44	110.70
2	A	207	NAP	O4B-C1B-C2B	-4.40	99.10	106.61
2	A	207	NAP	O7N-C7N-N7N	4.21	128.69	122.62
2	A	207	NAP	O2A-PA-O1A	3.98	130.98	112.44
2	A	207	NAP	C2D-C3D-C4D	-3.98	94.91	102.61
2	A	207	NAP	C2B-C3B-C4B	-3.84	93.73	101.99
2	A	207	NAP	C6N-N1N-C1D	-3.79	112.28	119.73
2	A	207	NAP	O3X-P2B-O2X	3.55	121.10	107.80
2	A	207	NAP	C5B-C4B-C3B	-3.50	102.62	115.21
3	A	307	COQ	C31-O3'-C3'	3.48	124.97	117.50
3	A	307	COQ	C2B-N3'-C4B	3.22	125.92	116.72
2	A	207	NAP	C3B-C2B-C1B	-3.19	96.69	102.81
2	A	207	NAP	C5N-C6N-N1N	2.98	124.45	120.38
2	A	207	NAP	O2B-P2B-O1X	-2.95	98.81	109.33
2	A	207	NAP	O2A-PA-O3	2.82	114.91	107.27
2	A	207	NAP	O2B-C2B-C1B	-2.66	100.71	110.05
3	A	307	COQ	C9'-C1'-C2'	2.62	125.20	120.27
2	A	207	NAP	O3B-C3B-C2B	2.58	118.40	111.19
2	A	207	NAP	PA-O5B-C5B	-2.51	106.99	121.35
2	A	207	NAP	C4N-C3N-C7N	-2.44	114.42	121.06
3	A	307	COQ	C5B-C4A-C4B	-2.41	122.57	124.75
3	A	307	COQ	N2'-C2B-N3'	-2.21	113.91	117.22
2	A	207	NAP	O5D-C5D-C4D	-2.18	101.56	108.99
3	A	307	COQ	N8'-C8A-N1'	2.16	118.12	115.77
3	A	307	COQ	C5B-C4A-C8A	2.16	119.97	118.11
2	A	207	NAP	C6N-N1N-C2N	-2.15	120.05	121.88

There are no chirality outliers.

All (9) torsion outliers are listed below:

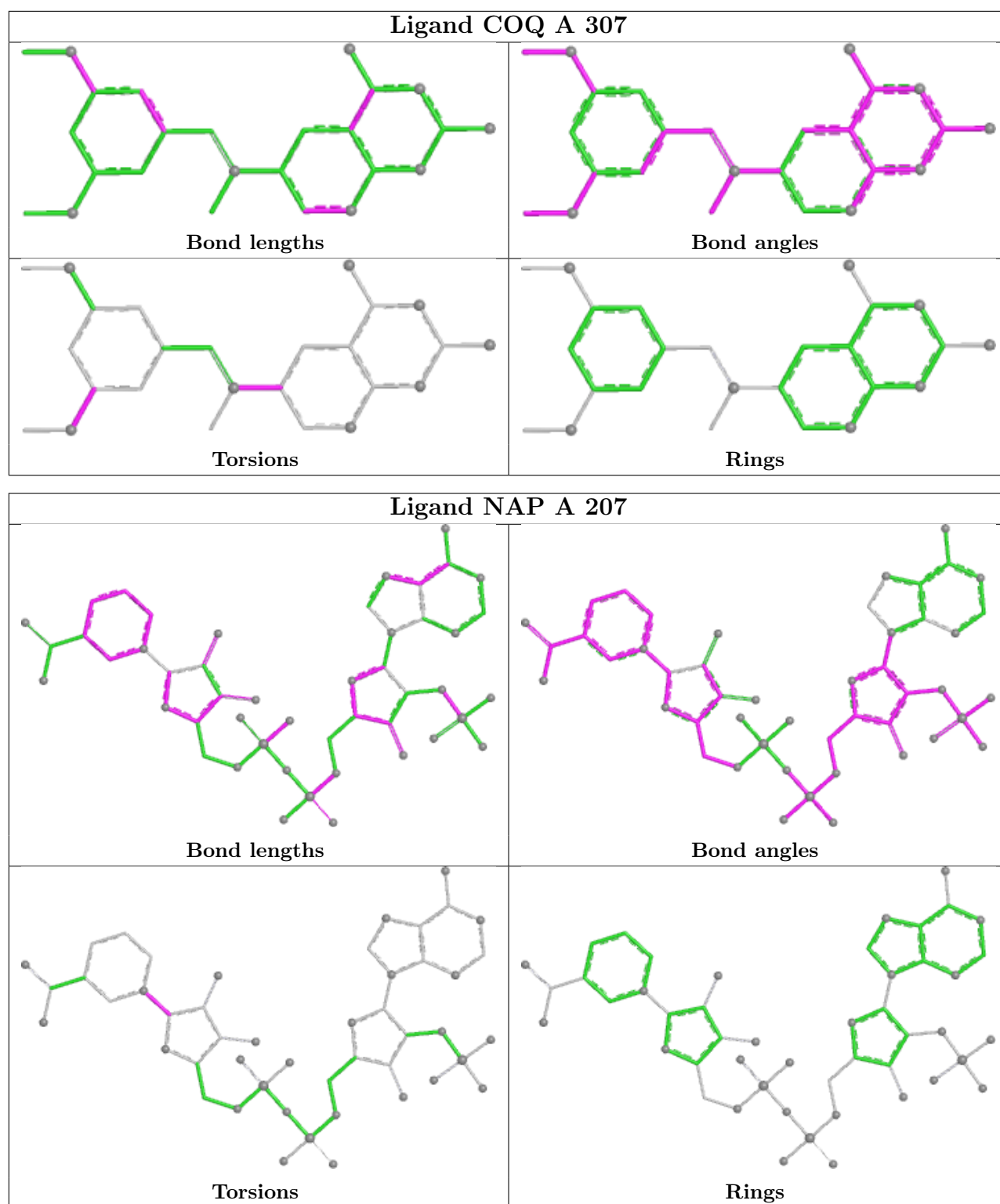
Mol	Chain	Res	Type	Atoms
2	A	207	NAP	O4D-C1D-N1N-C6N
2	A	207	NAP	C2D-C1D-N1N-C6N
3	A	307	COQ	C5B-C6B-N9'-C9'
3	A	307	COQ	C7'-C6B-N9'-C9'
3	A	307	COQ	C4'-C3'-O3'-C31
3	A	307	COQ	C2'-C3'-O3'-C31
3	A	307	COQ	C7'-C6B-N9'-CN'
3	A	307	COQ	C5B-C6B-N9'-CN'
2	A	207	NAP	O4D-C1D-N1N-C2N

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	307	COQ	3	0
2	A	207	NAP	10	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	205/206 (99%)	0.16	12 (5%)	22 27	11, 27, 52, 72	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ASN	4.8
1	A	90	ASN	4.3
1	A	91	GLY	3.8
1	A	86	LEU	3.6
1	A	69	PHE	3.1
1	A	46	PHE	2.7
1	A	48	SER	2.6
1	A	49	PHE	2.5
1	A	84	GLU	2.4
1	A	111	SER	2.4
1	A	112	GLU	2.3
1	A	195	PHE	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 monosaccharides in this entry.

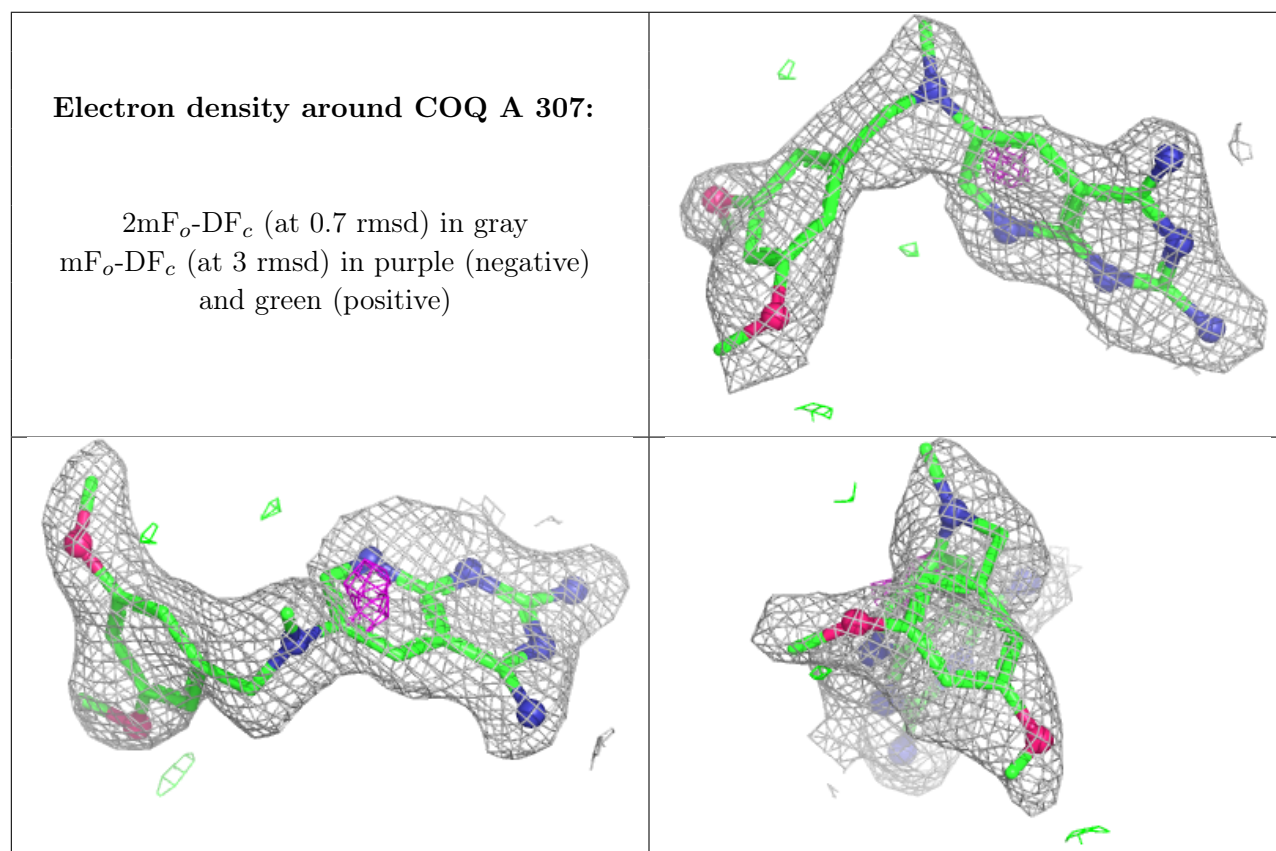
6.4 Ligands [i](#)

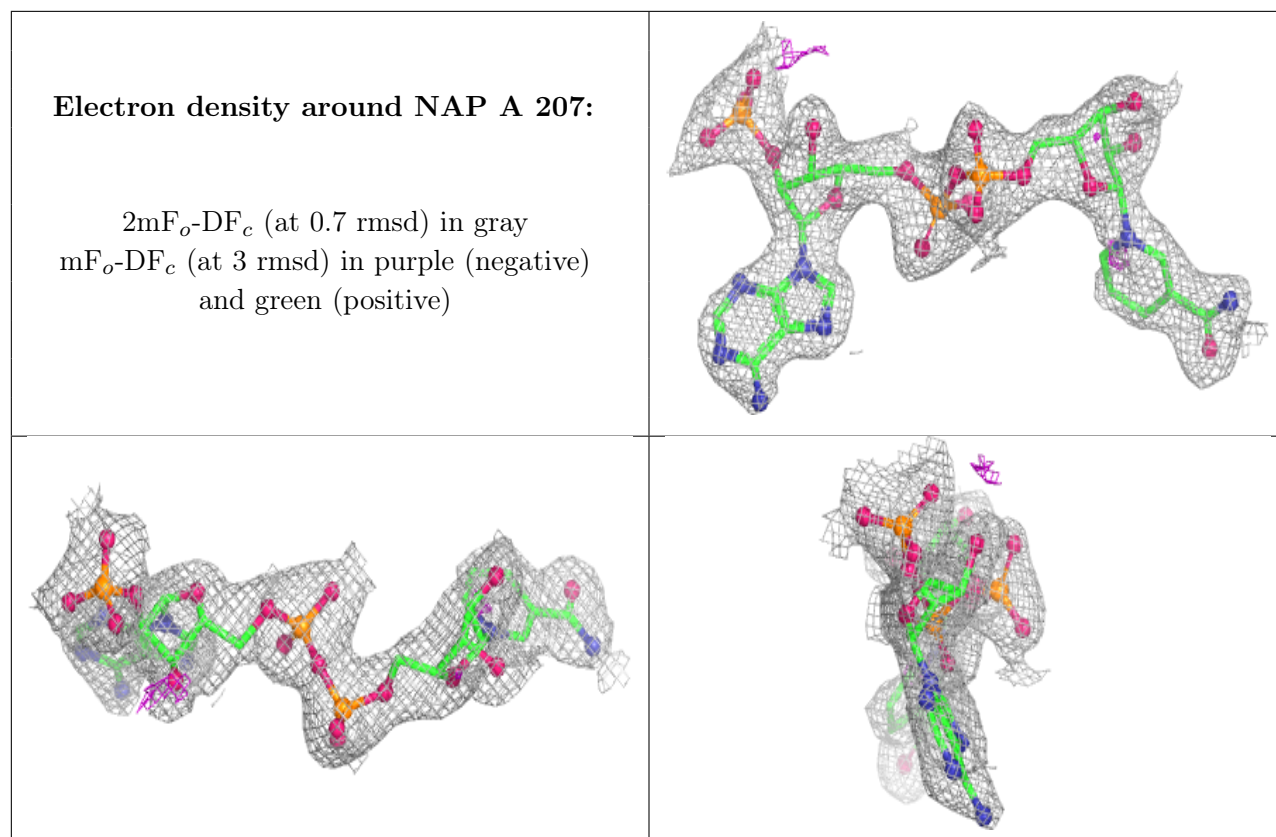
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	COQ	A	307	25/25	0.82	0.21	28,37,41,42	0
2	NAP	A	207	48/48	0.94	0.12	25,37,46,47	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.