



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:18 PM UTC

PDB ID : 1DAJ / pdb_00001daj
Title : COMPARISON OF TERNARY COMPLEXES OF PNEUMOCYSTIS CARINII AND WILD TYPE HUMAN DIHYDROFOLATE REDUCTASE WITH COENZYME NADPH AND A NOVEL CLASSICAL ANTITUMOR FURO[2,3D]PYRIMIDINE ANTIFOLATE
Authors : Cody, V.; Galitsky, N.; Luft, J.R.; Pangborn, W.; Gangjee, A.; Devraj, R.; Queener, S.F.; Blakley, R.L.
Deposited on : 1997-07-29
Resolution : 2.30 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

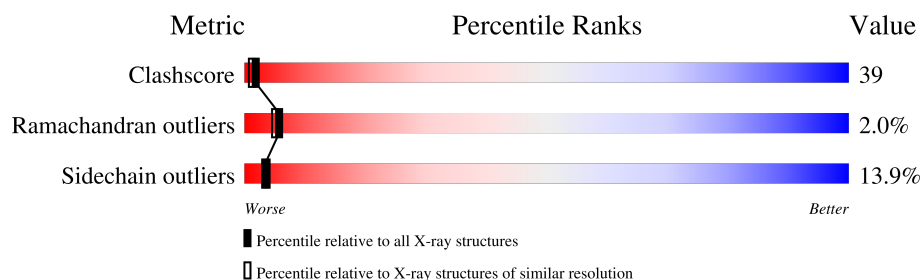
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	206	30% 47% 20% .

2 Entry composition [i](#)

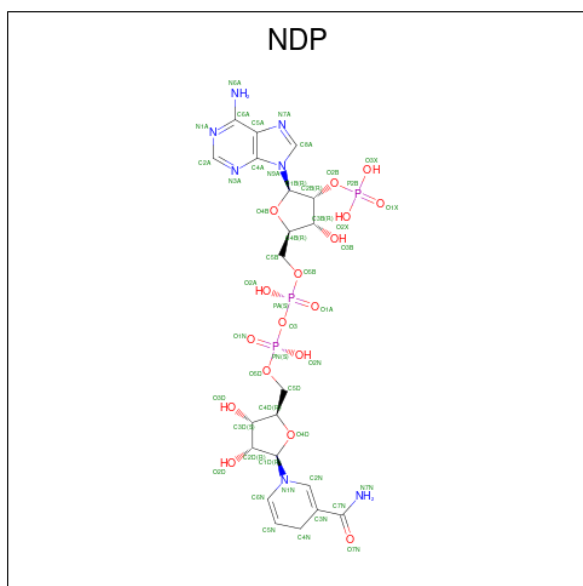
There are 4 unique types of molecules in this entry. The entry contains 1816 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

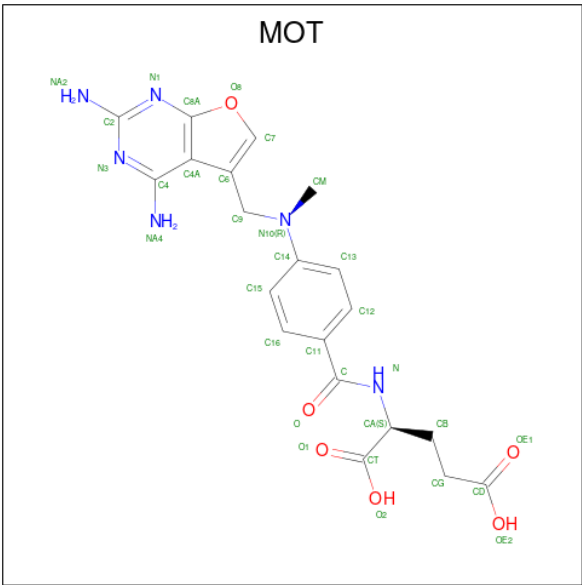
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	206	1686	1086	288	305	7	0	0	0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 3 is N-[4-[(2,4-DIAMINOFURO[2,3D]PYRIMIDIN-5-YL)METHYL]METHYLAMINO]-BENZOYL]-L-GLUTAMATE (CCD ID: MOT) (formula: $C_{20}H_{22}N_6O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	20	6	6		

- Molecule 4 is water.

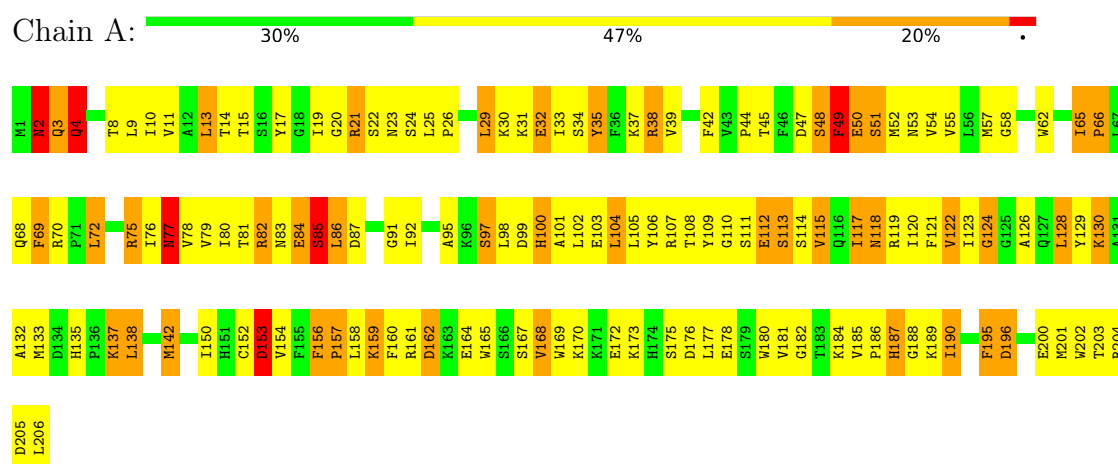
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: DIHYDROFOLATE REDUCTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	37.17Å 43.09Å 61.05Å 90.00° 94.85° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1816	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MOT, NDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.93	0/1728	2.10	69/2330 (3.0%)

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ASN	CA-CB-CG	13.34	125.94	112.60
1	A	75	ARG	CD-NE-CZ	9.80	138.12	124.40
1	A	85	SER	N-CA-C	-9.67	100.07	112.93
1	A	153	ASP	CA-CB-CG	9.62	122.22	112.60
1	A	87	ASP	N-CA-C	-9.15	98.73	110.53
1	A	159	LYS	CA-C-N	8.94	133.15	120.28
1	A	159	LYS	C-N-CA	8.94	133.15	120.28
1	A	160	PHE	CA-CB-CG	8.89	122.69	113.80
1	A	49	PHE	CA-CB-CG	-7.99	105.81	113.80
1	A	77	ASN	CA-CB-CG	7.79	120.39	112.60
1	A	35	TYR	N-CA-C	-7.69	102.83	111.14
1	A	157	PRO	N-CA-C	7.36	124.48	113.81
1	A	203	THR	N-CA-CB	7.29	124.38	111.69
1	A	83	ASN	CA-CB-CG	-7.15	105.45	112.60
1	A	21	ARG	CD-NE-CZ	7.14	134.39	124.40
1	A	51	SER	N-CA-C	6.97	121.21	110.20
1	A	100	HIS	N-CA-C	-6.72	104.03	111.36
1	A	32	GLU	N-CA-C	-6.62	104.14	111.36
1	A	84	GLU	N-CA-C	-6.55	98.55	108.96
1	A	58	GLY	N-CA-C	-6.54	103.80	112.82
1	A	132	ALA	N-CA-C	-6.37	103.85	111.69
1	A	65	ILE	O-C-N	6.33	127.08	121.57
1	A	38	ARG	CD-NE-CZ	6.12	132.97	124.40
1	A	87	ASP	CA-CB-CG	6.07	118.67	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	ASN	CA-CB-CG	6.05	118.65	112.60
1	A	162	ASP	CA-CB-CG	6.05	118.65	112.60
1	A	187	HIS	CA-C-O	-6.04	114.29	121.66
1	A	4	GLN	CB-CG-CD	6.02	122.83	112.60
1	A	72	LEU	CB-CA-C	5.99	119.25	109.90
1	A	69	PHE	N-CA-C	5.96	119.30	112.57
1	A	114	SER	N-CA-C	-5.95	106.00	113.20
1	A	187	HIS	N-CA-C	-5.94	101.22	110.42
1	A	50	GLU	CA-C-N	5.93	129.90	121.42
1	A	50	GLU	C-N-CA	5.93	129.90	121.42
1	A	8	THR	N-CA-C	-5.91	100.27	109.72
1	A	176	ASP	CA-CB-CG	-5.76	106.84	112.60
1	A	122	VAL	N-CA-C	-5.75	98.94	107.51
1	A	168	VAL	CA-C-O	5.75	127.97	120.78
1	A	87	ASP	CA-C-O	-5.73	115.35	121.94
1	A	31	LYS	N-CA-C	-5.72	106.14	113.23
1	A	138	LEU	CB-CA-C	5.71	119.75	110.22
1	A	97	SER	CA-C-N	5.67	128.44	120.28
1	A	97	SER	C-N-CA	5.67	128.44	120.28
1	A	79	VAL	N-CA-CB	-5.60	104.61	111.00
1	A	205	ASP	CA-C-O	-5.58	114.18	120.43
1	A	66	PRO	CB-CA-C	5.57	118.72	111.64
1	A	175	SER	O-C-N	5.53	128.00	122.08
1	A	85	SER	CA-C-O	5.50	127.50	120.07
1	A	82	ARG	N-CA-C	-5.50	104.93	111.69
1	A	115	VAL	CA-C-O	5.46	125.79	120.27
1	A	180	TRP	CA-C-N	5.41	129.83	121.34
1	A	180	TRP	C-N-CA	5.41	129.83	121.34
1	A	37	LYS	CA-CB-CG	5.34	124.78	114.10
1	A	42	PHE	CA-CB-CG	-5.34	108.46	113.80
1	A	156	PHE	CA-C-N	5.30	125.62	119.47
1	A	156	PHE	C-N-CA	5.30	125.62	119.47
1	A	162	ASP	CA-C-N	5.29	127.63	120.38
1	A	162	ASP	C-N-CA	5.29	127.63	120.38
1	A	9	LEU	N-CA-C	-5.26	101.30	109.72
1	A	124	GLY	CA-C-N	5.26	131.16	121.70
1	A	124	GLY	C-N-CA	5.26	131.16	121.70
1	A	142	MET	CA-C-O	-5.24	115.71	121.58
1	A	75	ARG	NE-CZ-NH1	5.20	126.70	121.50
1	A	14	THR	CA-CB-OG1	-5.19	101.82	109.60
1	A	142	MET	O-C-N	5.18	129.17	122.43
1	A	103	GLU	CB-CG-CD	5.15	121.35	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	VAL	N-CA-CB	-5.15	101.45	112.00
1	A	167	SER	N-CA-C	-5.08	107.47	113.97
1	A	196	ASP	N-CA-C	-5.07	100.98	109.24

There are no chirality outliers.

There are no planarity outliers.

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	1693	132	0
2	A	48	0	26	8	0
3	A	32	0	20	8	0
4	A	50	0	0	4	0
All	All	1816	0	1739	138	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 39.

All (138) 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)
2:A:207:NDP:H42N	3:A:208:MOT:H91	1.39	1.00
1:A:150:ILE:HD11	1:A:195:PHE:CE1	1.99	0.98
1:A:122:VAL:HG13	1:A:128:LEU:HD13	1.55	0.89
1:A:22:SER:H	1:A:153:ASP:CG	1.81	0.89
1:A:178:GLU:HG2	1:A:184:LYS:HA	1.54	0.86
1:A:22:SER:N	1:A:153:ASP:OD1	2.10	0.85
1:A:122:VAL:HG13	1:A:128:LEU:CD1	2.09	0.82
1:A:130:LYS:HG3	1:A:157:PRO:HB3	1.62	0.82
1:A:3:GLN:HB3	1:A:137:LYS:HD3	1.62	0.81
1:A:3:GLN:HB3	1:A:137:LYS:CD	2.11	0.80
1:A:104:LEU:HD12	1:A:108:THR:HG1	1.48	0.79
1:A:54:VAL:HB	1:A:120:ILE:HD13	1.65	0.79
1:A:104:LEU:HD12	1:A:108:THR:OG1	1.84	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LEU:HB3	1:A:32:GLU:HB3	1.67	0.76
1:A:85:SER:HB2	1:A:86:LEU:HD13	1.69	0.74
1:A:81:THR:HG23	1:A:84:GLU:HB3	1.69	0.73
1:A:54:VAL:HG23	1:A:117:ILE:HG21	1.71	0.72
1:A:54:VAL:HG23	1:A:117:ILE:CG2	2.19	0.72
1:A:69:PHE:CG	3:A:208:MOT:HB2	2.25	0.71
1:A:4:GLN:HB3	4:A:257:HOH:O	1.91	0.70
1:A:177:LEU:C	1:A:177:LEU:HD23	2.16	0.70
1:A:13:LEU:HD12	1:A:17:TYR:HA	1.73	0.70
1:A:122:VAL:CG1	1:A:128:LEU:HD13	2.22	0.69
1:A:137:LYS:HA	1:A:137:LYS:HE3	1.73	0.69
1:A:150:ILE:HD11	1:A:195:PHE:HE1	1.51	0.69
1:A:133:MET:HE3	1:A:158:LEU:HD22	1.75	0.69
1:A:104:LEU:HD12	1:A:104:LEU:O	1.93	0.69
1:A:161:ARG:HD3	4:A:233:HOH:O	1.94	0.67
2:A:207:NDP:H8A	2:A:207:NDP:H52A	1.75	0.67
1:A:78:VAL:HG21	1:A:105:LEU:HD21	1.79	0.64
1:A:173:LYS:HG3	4:A:229:HOH:O	1.97	0.64
1:A:29:LEU:HB3	1:A:32:GLU:CB	2.30	0.60
1:A:200:GLU:OE1	1:A:202:TRP:NE1	2.34	0.60
1:A:52:MET:O	1:A:117:ILE:HA	2.02	0.60
1:A:57:MET:HE2	1:A:123:ILE:HD11	1.83	0.60
1:A:66:PRO:HB2	1:A:69:PHE:CD2	2.38	0.59
1:A:164:GLU:HG3	1:A:165:TRP:CD1	2.37	0.59
1:A:45:THR:HA	1:A:48:SER:OG	2.03	0.59
1:A:135:HIS:HD2	1:A:137:LYS:H	1.51	0.59
1:A:54:VAL:CG2	1:A:117:ILE:HG21	2.33	0.58
1:A:186:PRO:HB2	1:A:190:ILE:HD11	1.86	0.58
1:A:126:ALA:HB2	1:A:154:VAL:CG2	2.33	0.58
1:A:150:ILE:HD11	1:A:195:PHE:CD1	2.40	0.56
1:A:77:ASN:N	1:A:77:ASN:HD22	2.03	0.56
1:A:104:LEU:CD1	1:A:108:THR:OG1	2.53	0.56
1:A:19:ILE:HG13	1:A:154:VAL:HG13	1.87	0.56
1:A:23:ASN:HA	2:A:207:NDP:H3D	1.89	0.55
1:A:110:GLY:O	1:A:112:GLU:N	2.40	0.55
1:A:47:ASP:C	1:A:49:PHE:H	2.15	0.54
1:A:104:LEU:HD12	1:A:104:LEU:C	2.32	0.54
2:A:207:NDP:H42N	3:A:208:MOT:C9	2.27	0.54
1:A:84:GLU:CD	1:A:84:GLU:O	2.51	0.54
1:A:54:VAL:HG22	1:A:76:ILE:HB	1.88	0.54
1:A:54:VAL:HB	1:A:120:ILE:CD1	2.37	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LYS:HE3	1:A:137:LYS:CA	2.34	0.53
1:A:3:GLN:HG2	1:A:137:LYS:HG3	1.92	0.52
1:A:178:GLU:OE2	1:A:184:LYS:HG3	2.09	0.52
1:A:80:ILE:O	2:A:207:NDP:H1B	2.10	0.52
1:A:80:ILE:CD1	1:A:101:ALA:HB2	2.40	0.51
1:A:47:ASP:C	1:A:49:PHE:N	2.68	0.51
1:A:97:SER:OG	1:A:100:HIS:HD2	1.94	0.51
1:A:169:TRP:CH2	1:A:204:ARG:HG2	2.45	0.51
1:A:126:ALA:HB2	1:A:154:VAL:HG21	1.91	0.51
1:A:10:ILE:HA	1:A:142:MET:O	2.11	0.51
1:A:24:SER:O	1:A:26:PRO:HD3	2.10	0.51
1:A:35:TYR:O	1:A:38:ARG:HB3	2.11	0.50
1:A:50:GLU:HG2	1:A:51:SER:N	2.27	0.50
1:A:19:ILE:O	2:A:207:NDP:H2N	2.12	0.50
1:A:82:ARG:HG2	2:A:207:NDP:H2A	1.93	0.50
1:A:172:GLU:HG3	1:A:201:MET:HE3	1.92	0.50
1:A:35:TYR:O	1:A:39:VAL:HG23	2.11	0.50
3:A:208:MOT:O	3:A:208:MOT:CB	2.55	0.50
1:A:78:VAL:CG2	1:A:105:LEU:HD21	2.42	0.49
1:A:21:ARG:HD2	1:A:153:ASP:OD2	2.12	0.49
1:A:72:LEU:HB3	1:A:75:ARG:CZ	2.43	0.49
1:A:66:PRO:O	1:A:69:PHE:N	2.45	0.49
1:A:98:LEU:O	1:A:102:LEU:HG	2.13	0.49
1:A:4:GLN:HG2	1:A:106:TYR:CE2	2.47	0.48
1:A:54:VAL:O	1:A:121:PHE:N	2.41	0.48
1:A:85:SER:C	1:A:86:LEU:HD13	2.38	0.48
1:A:170:LYS:O	1:A:202:TRP:HA	2.13	0.48
1:A:65:ILE:HG22	1:A:70:ARG:HG3	1.95	0.48
1:A:113:SER:C	1:A:115:VAL:H	2.20	0.48
1:A:187:HIS:CD2	1:A:188:GLY:H	2.31	0.48
1:A:69:PHE:CB	3:A:208:MOT:HB2	2.43	0.48
1:A:17:TYR:CE2	1:A:159:LYS:HA	2.49	0.47
1:A:65:ILE:CG2	1:A:70:ARG:HG3	2.45	0.47
1:A:105:LEU:O	1:A:109:TYR:N	2.47	0.47
1:A:54:VAL:N	1:A:119:ARG:O	2.42	0.46
1:A:47:ASP:O	1:A:49:PHE:N	2.49	0.46
1:A:85:SER:CB	1:A:86:LEU:HD13	2.44	0.46
1:A:22:SER:N	1:A:153:ASP:OD2	2.48	0.46
1:A:159:LYS:HD3	1:A:162:ASP:OD2	2.16	0.46
1:A:3:GLN:HB3	1:A:137:LYS:HD2	1.95	0.46
1:A:133:MET:CE	1:A:158:LEU:HD22	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ALA:HB2	1:A:101:ALA:HA	1.99	0.45
1:A:54:VAL:HG23	1:A:117:ILE:HG23	1.96	0.45
1:A:142:MET:SD	1:A:201:MET:HG3	2.57	0.45
1:A:53:ASN:OD1	1:A:119:ARG:HB2	2.17	0.45
1:A:185:VAL:CG1	1:A:186:PRO:HD2	2.47	0.44
1:A:4:GLN:HG2	1:A:106:TYR:CZ	2.53	0.44
1:A:77:ASN:N	1:A:77:ASN:ND2	2.65	0.44
1:A:86:LEU:HD13	1:A:86:LEU:N	2.32	0.44
1:A:168:VAL:HB	1:A:169:TRP:H	1.58	0.44
1:A:177:LEU:HD23	1:A:178:GLU:N	2.32	0.44
1:A:34:SER:O	1:A:38:ARG:HB2	2.18	0.44
1:A:44:PRO:HD3	4:A:235:HOH:O	2.16	0.44
1:A:69:PHE:HB3	3:A:208:MOT:HB2	1.99	0.44
1:A:126:ALA:HB2	1:A:154:VAL:HG22	1.99	0.44
3:A:208:MOT:HM1	3:A:208:MOT:H15	1.78	0.43
1:A:32:GLU:O	1:A:35:TYR:HB3	2.18	0.43
1:A:156:PHE:HA	1:A:157:PRO:HD2	1.70	0.43
1:A:187:HIS:HD2	1:A:188:GLY:H	1.66	0.43
1:A:69:PHE:HB3	3:A:208:MOT:HA	2.00	0.43
1:A:85:SER:C	1:A:86:LEU:CD1	2.91	0.43
2:A:207:NDP:H52A	2:A:207:NDP:C8A	2.47	0.43
1:A:66:PRO:C	1:A:68:GLN:N	2.76	0.43
1:A:185:VAL:HG12	1:A:186:PRO:HD2	2.01	0.43
1:A:62:TRP:CE2	1:A:70:ARG:HD3	2.53	0.43
1:A:129:TYR:O	1:A:133:MET:HG2	2.20	0.42
1:A:95:ALA:CB	1:A:101:ALA:HA	2.49	0.42
1:A:29:LEU:HD11	1:A:195:PHE:HD2	1.85	0.42
1:A:99:ASP:OD1	1:A:135:HIS:HE1	2.02	0.42
1:A:150:ILE:CD1	1:A:195:PHE:CE1	2.89	0.42
1:A:57:MET:HA	1:A:124:GLY:O	2.19	0.42
1:A:107:ARG:HH11	1:A:107:ARG:HD3	1.61	0.42
1:A:38:ARG:HB2	1:A:38:ARG:HE	1.13	0.42
1:A:126:ALA:CB	1:A:154:VAL:HG21	2.50	0.42
1:A:126:ALA:CB	1:A:154:VAL:CG2	2.97	0.42
1:A:20:GLY:O	1:A:152:CYS:HB3	2.20	0.41
1:A:82:ARG:HG3	1:A:82:ARG:NH1	2.34	0.41
1:A:91:GLY:C	1:A:92:ILE:HD12	2.46	0.41
1:A:82:ARG:C	1:A:84:GLU:H	2.28	0.41
1:A:25:LEU:HD23	1:A:25:LEU:HA	1.66	0.41
1:A:181:VAL:O	1:A:181:VAL:CG1	2.69	0.41
1:A:110:GLY:O	1:A:113:SER:N	2.42	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LYS:HD2	1:A:196:ASP:OD1	2.22	0.40
1:A:156:PHE:CD1	1:A:158:LEU:O	2.75	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	204/206 (99%)	183 (90%)	17 (8%)	4 (2%)	6 5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	SER
1	A	2	ASN
1	A	48	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	187/187 (100%)	161 (86%)	26 (14%)	3 4

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	3	GLN
1	A	4	GLN
1	A	13	LEU
1	A	15	THR
1	A	29	LEU
1	A	30	LYS
1	A	33	ILE
1	A	49	PHE
1	A	55	VAL
1	A	77	ASN
1	A	85	SER
1	A	86	LEU
1	A	104	LEU
1	A	112	GLU
1	A	113	SER
1	A	117	ILE
1	A	118	ASN
1	A	128	LEU
1	A	130	LYS
1	A	137	LYS
1	A	138	LEU
1	A	153	ASP
1	A	190	ILE
1	A	195	PHE
1	A	206	LEU

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	83	ASN
1	A	100	HIS
1	A	118	ASN
1	A	135	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 [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](#)

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	NDP	A	207	-	51,52,52	2.55	17 (33%)	71,80,80	2.01	28 (39%)
3	MOT	A	208	-	34,34,34	3.37	16 (47%)	41,48,48	2.89	17 (41%)

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	NDP	A	207	-	-	5/34/77/77	0/5/5/5
3	MOT	A	208	-	-	4/25/25/25	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	208	MOT	O8-C8A	-10.45	1.23	1.37
2	A	207	NDP	O4B-C4B	-8.39	1.26	1.45
2	A	207	NDP	P2B-O2B	7.83	1.73	1.59
3	A	208	MOT	C4A-C4	-7.64	1.33	1.42
3	A	208	MOT	C11-C	-7.02	1.34	1.50
3	A	208	MOT	C4A-C8A	-6.06	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	207	NDP	C5A-C6A	5.62	1.56	1.41
3	A	208	MOT	C4-N3	-5.08	1.28	1.35
3	A	208	MOT	O8-C7	-4.93	1.24	1.38
2	A	207	NDP	C5A-C4A	-4.30	1.31	1.39
2	A	207	NDP	C3B-C4B	4.15	1.63	1.53
3	A	208	MOT	C2-N3	-3.56	1.29	1.35
2	A	207	NDP	PN-O5D	-3.47	1.45	1.59
2	A	207	NDP	O3B-C3B	3.28	1.51	1.43
2	A	207	NDP	C4N-C3N	3.26	1.56	1.50
2	A	207	NDP	C5A-N7A	3.05	1.44	1.39
2	A	207	NDP	C4A-N9A	-3.03	1.31	1.37
2	A	207	NDP	C1D-N1N	2.85	1.54	1.46
3	A	208	MOT	C13-C12	-2.81	1.34	1.38
3	A	208	MOT	C16-C11	-2.71	1.35	1.39
2	A	207	NDP	PA-O5B	2.67	1.69	1.59
2	A	207	NDP	PN-O1N	-2.59	1.41	1.50
2	A	207	NDP	P2B-O2X	-2.55	1.45	1.54
3	A	208	MOT	C16-C15	-2.53	1.34	1.38
3	A	208	MOT	OE2-CD	-2.51	1.22	1.30
3	A	208	MOT	C13-C14	-2.43	1.34	1.39
3	A	208	MOT	CA-N	2.37	1.50	1.45
3	A	208	MOT	O2-CT	-2.35	1.23	1.30
3	A	208	MOT	C15-C14	-2.27	1.35	1.39
2	A	207	NDP	PA-O3	-2.25	1.57	1.59
3	A	208	MOT	C12-C11	-2.17	1.36	1.39
2	A	207	NDP	O2B-C2B	-2.11	1.36	1.44
2	A	207	NDP	O4D-C4D	2.08	1.49	1.45

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	208	MOT	O8-C8A-N1	9.08	124.03	119.20
3	A	208	MOT	CA-N-C	-5.94	107.31	121.56
3	A	208	MOT	C8A-O8-C7	5.50	109.31	105.80
3	A	208	MOT	C2-N3-C4	5.33	123.68	117.28
3	A	208	MOT	C4A-C6-C7	-4.96	101.14	105.34
2	A	207	NDP	O4B-C1B-C2B	-4.90	98.15	106.59
3	A	208	MOT	O8-C8A-C4A	4.82	113.11	110.00
2	A	207	NDP	O3X-P2B-O2X	4.50	124.67	107.80
3	A	208	MOT	O-C-N	-3.99	114.88	122.47
2	A	207	NDP	O3B-C3B-C4B	-3.95	99.74	111.08
2	A	207	NDP	O7N-C7N-C3N	-3.81	113.71	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	207	NDP	C3N-C2N-N1N	-3.71	117.75	123.20
2	A	207	NDP	C2B-C3B-C4B	-3.55	94.37	101.99
3	A	208	MOT	O2-CT-O1	-3.52	116.09	124.08
2	A	207	NDP	O2A-PA-O3	3.42	116.52	107.27
3	A	208	MOT	C4A-C4-N3	-3.40	115.77	121.62
2	A	207	NDP	N3A-C2A-N1A	3.17	133.38	128.58
2	A	207	NDP	O5D-C5D-C4D	-3.13	98.35	108.99
3	A	208	MOT	NA4-C4-N3	3.08	121.19	117.03
2	A	207	NDP	C3B-C2B-C1B	-3.06	96.96	102.81
3	A	208	MOT	CB-CA-CT	3.02	117.52	110.35
2	A	207	NDP	C3N-C7N-N7N	2.95	122.91	117.67
2	A	207	NDP	C4B-O4B-C1B	2.94	115.95	109.47
2	A	207	NDP	C1D-N1N-C6N	-2.72	115.03	120.77
2	A	207	NDP	O4B-C1B-N9A	2.63	113.15	108.09
2	A	207	NDP	C2A-N1A-C6A	-2.60	114.46	118.73
3	A	208	MOT	CG-CB-CA	2.53	117.82	113.16
2	A	207	NDP	C4A-N9A-C8A	2.49	108.35	105.74
3	A	208	MOT	C2-N1-C8A	-2.47	112.52	115.96
2	A	207	NDP	C6N-N1N-C2N	2.47	121.96	119.32
2	A	207	NDP	O2B-P2B-O1X	-2.45	100.61	109.33
2	A	207	NDP	C5B-C4B-C3B	-2.44	106.43	115.21
2	A	207	NDP	P2B-O2B-C2B	-2.38	117.07	123.43
2	A	207	NDP	O5B-C5B-C4B	-2.34	101.03	108.99
3	A	208	MOT	O2-CT-CA	2.28	121.22	113.51
2	A	207	NDP	N6A-C6A-N1A	2.28	123.45	118.38
2	A	207	NDP	C2D-C3D-C4D	-2.27	98.23	102.61
3	A	208	MOT	NA2-C2-N3	2.26	120.61	117.22
2	A	207	NDP	O2A-PA-O1A	2.26	122.95	112.44
3	A	208	MOT	C13-C14-N10	2.24	124.71	121.59
2	A	207	NDP	O4D-C1D-N1N	2.19	112.27	108.08
2	A	207	NDP	O5B-PA-O1A	-2.04	100.84	108.94
3	A	208	MOT	C11-C-N	2.04	120.82	117.04
2	A	207	NDP	O5D-PN-O1N	2.04	117.00	108.94
2	A	207	NDP	C5A-N7A-C8A	-2.02	100.27	103.45

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	208	MOT	N-CA-CB-CG
3	A	208	MOT	CT-CA-CB-CG
2	A	207	NDP	PN-O3-PA-O1A

Continued on next page...

Continued from previous page...

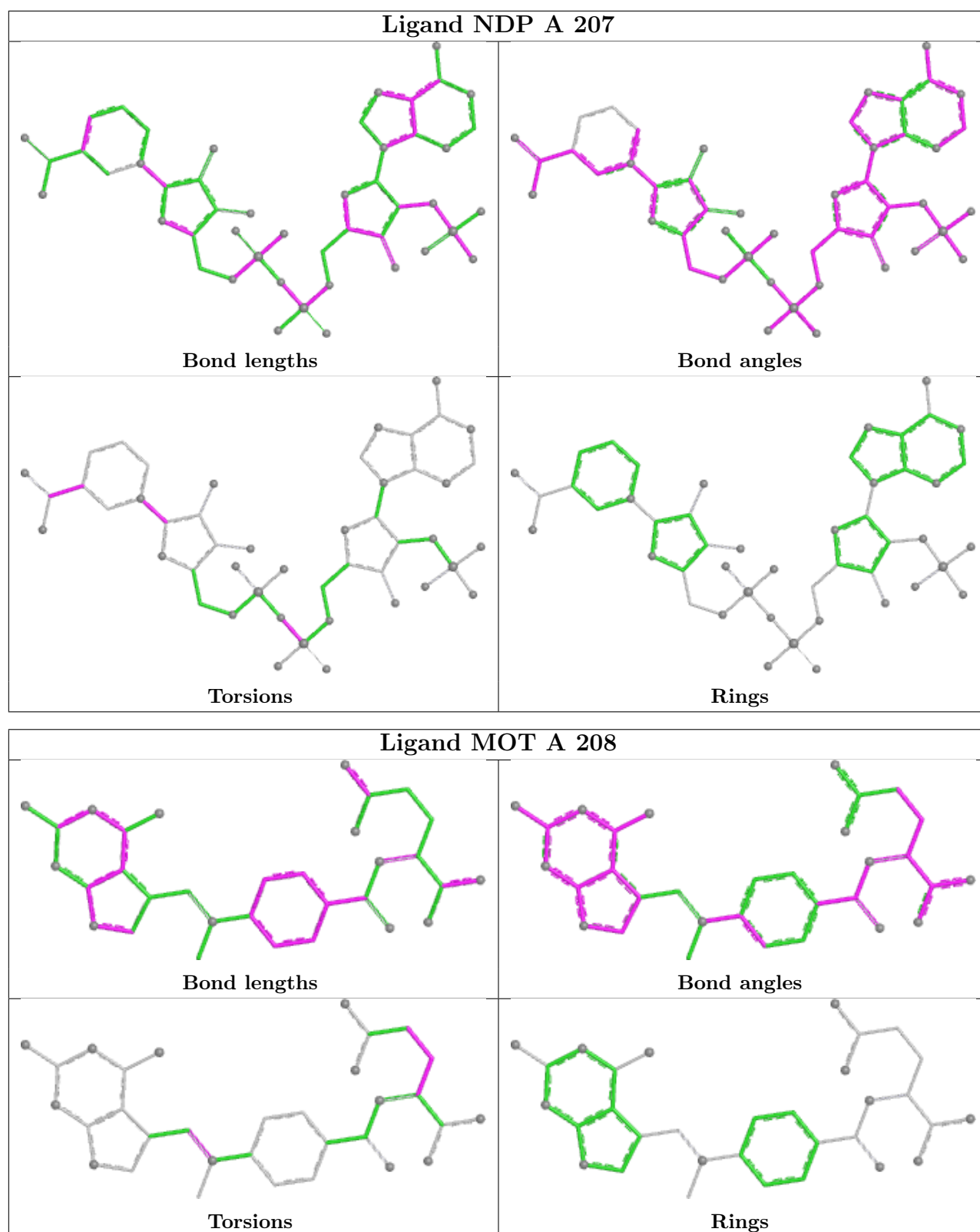
Mol	Chain	Res	Type	Atoms
2	A	207	NDP	PN-O3-PA-O2A
3	A	208	MOT	CA-CB-CG-CD
2	A	207	NDP	O4D-C1D-N1N-C2N
2	A	207	NDP	C2N-C3N-C7N-N7N
2	A	207	NDP	C2D-C1D-N1N-C2N
3	A	208	MOT	C6-C9-N10-C14

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	207	NDP	8	0
3	A	208	MOT	8	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.