



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:05 PM UTC

PDB ID : 1HFP / pdb_00001hfp
Title : COMPARISON OF TERNARY CRYSTAL COMPLEXES OF HUMAN DI-HYDROFOLATE REDUCTASE WITH NADPH AND A CLASSICAL AN-TITUMOR FUOPYRIMDINE
Authors : Cody, V.; Galitsky, N.; Luft, J.R.; Pangborn, W.; Blakley, R.L.; Gangjee, A.
Deposited on : 1997-11-04
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	:	4-5-2 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

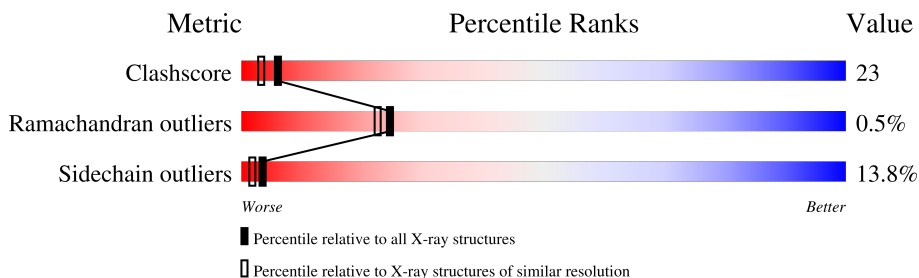
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	186	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1622 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.

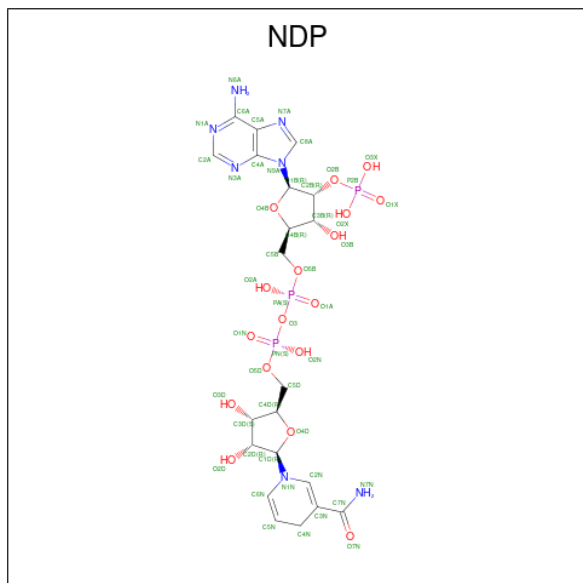
- Molecule 1 is a protein called DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1495	956	253	279	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

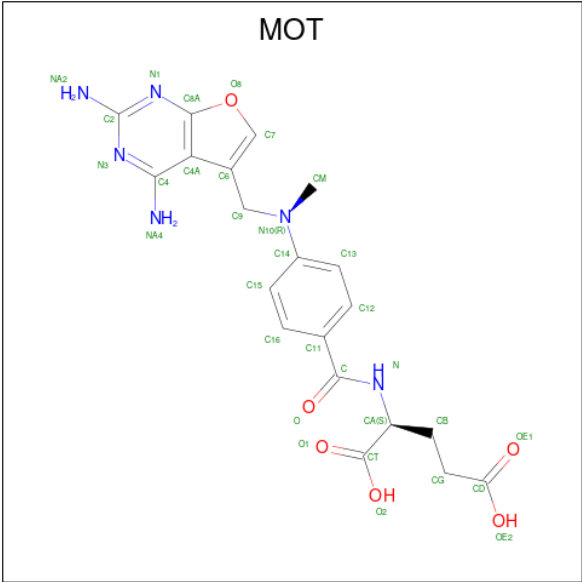
Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLY	PHE	engineered mutation	UNP P00374

- 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.

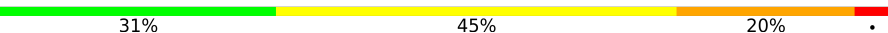
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		

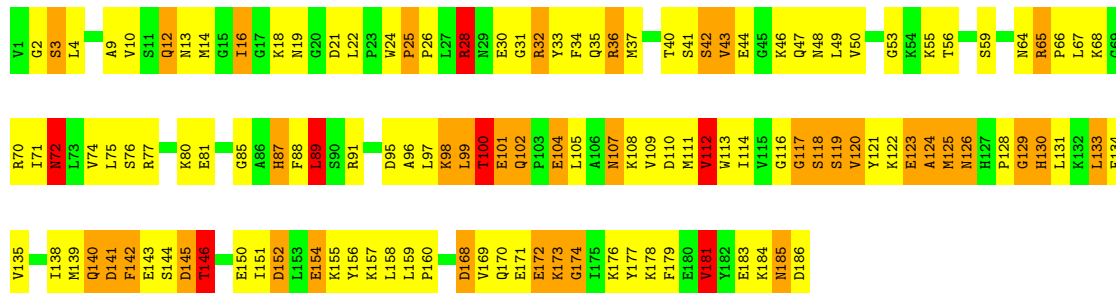
3 Residue-property plots

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

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	87.12Å 87.12Å 77.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	0.06	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	1622	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.43	6/1529 (0.4%)	3.06	171/2062 (8.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	GLY	N-CA	-11.34	1.35	1.45
1	A	116	GLY	C-N	-6.68	1.24	1.32
1	A	77	ARG	NE-CZ	6.59	1.40	1.33
1	A	56	THR	CA-CB	5.63	1.62	1.53
1	A	67	LEU	N-CA	5.57	1.53	1.46
1	A	119	SER	CB-OG	5.29	1.52	1.42

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	GLY	CA-C-N	39.12	179.75	122.64
1	A	116	GLY	C-N-CA	39.12	179.75	122.64
1	A	126	ASN	CA-CB-CG	15.82	128.42	112.60
1	A	116	GLY	N-CA-C	13.37	125.68	112.04
1	A	19	ASN	OD1-CG-ND2	-12.37	110.23	122.60
1	A	77	ARG	CD-NE-CZ	-10.71	109.40	124.40
1	A	185	ASN	CA-CB-CG	10.32	122.92	112.60
1	A	141	ASP	CA-CB-CG	-10.29	102.31	112.60
1	A	118	SER	CA-C-N	10.22	134.34	120.54
1	A	118	SER	C-N-CA	10.22	134.34	120.54
1	A	138	ILE	CB-CG1-CD1	9.78	134.33	113.80
1	A	77	ARG	CG-CD-NE	9.61	133.14	112.00
1	A	140	GLN	N-CA-CB	9.44	125.99	111.46
1	A	119	SER	CA-C-N	9.34	132.52	120.56
1	A	119	SER	C-N-CA	9.34	132.52	120.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	THR	CA-CB-OG1	-8.73	96.50	109.60
1	A	44	GLU	CA-C-O	8.68	130.82	120.92
1	A	44	GLU	CB-CG-CD	8.68	127.36	112.60
1	A	172	GLU	CA-CB-CG	8.54	131.18	114.10
1	A	119	SER	CA-C-O	8.19	129.67	120.90
1	A	32	ARG	NE-CZ-NH1	-8.14	113.36	121.50
1	A	181	VAL	CA-CB-CG2	8.14	124.25	110.40
1	A	177	TYR	CA-C-O	-8.05	112.64	121.33
1	A	126	ASN	OD1-CG-ND2	-8.04	114.56	122.60
1	A	101	GLU	CA-CB-CG	7.96	130.01	114.10
1	A	171	GLU	O-C-N	7.85	133.10	123.44
1	A	47	GLN	CB-CG-CD	-7.78	99.38	112.60
1	A	30	GLU	CA-C-N	7.75	128.59	119.98
1	A	30	GLU	C-N-CA	7.75	128.59	119.98
1	A	91	ARG	NE-CZ-NH2	7.67	126.11	119.20
1	A	9	ALA	CA-C-O	-7.63	112.14	120.30
1	A	146	THR	CB-CA-C	7.60	124.40	109.35
1	A	13	ASN	CA-CB-CG	7.59	120.19	112.60
1	A	75	LEU	CA-C-O	7.51	128.61	120.43
1	A	13	ASN	OD1-CG-ND2	-7.49	115.11	122.60
1	A	72	ASN	CB-CG-ND2	7.39	127.48	116.40
1	A	109	VAL	N-CA-C	7.32	118.82	108.36
1	A	65	ARG	CD-NE-CZ	7.18	134.45	124.40
1	A	151	ILE	CA-C-O	-7.06	112.74	120.71
1	A	172	GLU	CB-CG-CD	7.02	124.53	112.60
1	A	181	VAL	CB-CA-C	7.02	119.89	110.42
1	A	76	SER	CA-C-N	-6.94	110.25	122.26
1	A	76	SER	C-N-CA	-6.94	110.25	122.26
1	A	12	GLN	CA-CB-CG	-6.93	100.25	114.10
1	A	173	LYS	CB-CA-C	-6.90	100.50	111.48
1	A	12	GLN	OE1-CD-NE2	6.90	129.50	122.60
1	A	72	ASN	CA-CB-CG	6.88	119.48	112.60
1	A	2	GLY	CA-C-N	6.86	130.60	120.87
1	A	2	GLY	C-N-CA	6.86	130.60	120.87
1	A	126	ASN	CB-CG-OD1	6.79	134.38	120.80
1	A	102	GLN	N-CA-C	-6.77	101.25	109.72
1	A	85	GLY	CA-C-N	6.73	131.50	120.94
1	A	85	GLY	C-N-CA	6.73	131.50	120.94
1	A	174	GLY	O-C-N	6.71	129.66	122.41
1	A	49	LEU	CA-C-O	-6.70	113.12	120.43
1	A	160	PRO	CB-CA-C	6.70	122.10	111.31
1	A	3	SER	CA-CB-OG	-6.63	97.84	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	PHE	CA-C-O	6.63	128.00	120.90
1	A	139	MET	N-CA-C	6.58	119.82	110.68
1	A	112	VAL	CB-CA-C	6.57	120.56	110.96
1	A	3	SER	CA-C-O	-6.55	113.83	121.16
1	A	30	GLU	CB-CG-CD	6.53	123.70	112.60
1	A	124	ALA	N-CA-CB	6.44	119.72	110.06
1	A	154	GLU	N-CA-CB	6.43	120.89	110.40
1	A	154	GLU	N-CA-C	-6.41	104.94	112.89
1	A	65	ARG	NH1-CZ-NH2	-6.38	111.01	119.30
1	A	70	ARG	CA-C-O	-6.37	113.66	121.11
1	A	138	ILE	CA-CB-CG1	6.36	121.21	110.40
1	A	120	VAL	CB-CA-C	6.34	120.33	112.02
1	A	77	ARG	NE-CZ-NH2	6.34	124.91	119.20
1	A	145	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	64	ASN	CA-C-O	-6.28	112.31	119.78
1	A	87	HIS	ND1-CE1-NE2	-6.28	102.12	108.40
1	A	119	SER	O-C-N	-6.25	115.59	122.09
1	A	70	ARG	NE-CZ-NH2	-6.22	113.60	119.20
1	A	123	GLU	N-CA-CB	-6.21	101.07	110.07
1	A	181	VAL	N-CA-CB	6.17	120.22	111.82
1	A	112	VAL	CA-CB-CG1	6.16	120.88	110.40
1	A	118	SER	CA-C-O	6.09	127.00	120.55
1	A	59	SER	O-C-N	-6.06	114.01	122.37
1	A	71	ILE	CA-C-O	-6.03	113.60	120.65
1	A	129	GLY	O-C-N	6.01	128.95	123.00
1	A	138	ILE	N-CA-C	-5.93	99.16	108.23
1	A	113	TRP	CA-C-N	5.93	129.90	122.43
1	A	113	TRP	C-N-CA	5.93	129.90	122.43
1	A	101	GLU	CB-CA-C	-5.90	99.87	110.37
1	A	21	ASP	CA-CB-CG	-5.88	106.72	112.60
1	A	124	ALA	CA-C-N	5.86	128.94	120.38
1	A	124	ALA	C-N-CA	5.86	128.94	120.38
1	A	173	LYS	O-C-N	5.84	133.15	122.11
1	A	177	TYR	CA-CB-CG	5.81	124.35	113.90
1	A	81	GLU	CA-CB-CG	5.79	125.69	114.10
1	A	99	LEU	CA-C-N	5.77	128.48	120.29
1	A	99	LEU	C-N-CA	5.77	128.48	120.29
1	A	116	GLY	CA-C-O	-5.77	118.30	122.45
1	A	81	GLU	CG-CD-OE1	5.74	131.60	118.40
1	A	43	VAL	N-CA-C	5.72	116.52	108.17
1	A	157	LYS	CA-C-N	5.72	129.47	121.24
1	A	157	LYS	C-N-CA	5.72	129.47	121.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	LEU	CA-C-O	5.68	126.52	120.10
1	A	176	LYS	O-C-N	5.67	129.73	123.16
1	A	142	PHE	CA-C-O	-5.66	113.31	120.28
1	A	30	GLU	CA-C-O	5.66	126.42	120.42
1	A	177	TYR	O-C-N	5.64	129.68	123.25
1	A	16	ILE	CA-C-O	-5.64	113.94	118.90
1	A	141	ASP	O-C-N	5.63	129.70	123.16
1	A	144	SER	CA-CB-OG	-5.63	99.84	111.10
1	A	130	HIS	CA-CB-CG	-5.60	108.20	113.80
1	A	131	LEU	O-C-N	-5.60	117.00	123.33
1	A	169	VAL	CA-CB-CG2	5.58	119.89	110.40
1	A	3	SER	N-CA-C	5.56	118.52	110.28
1	A	179	PHE	CA-C-N	5.56	131.29	122.62
1	A	179	PHE	C-N-CA	5.56	131.29	122.62
1	A	88	PHE	O-C-N	5.55	129.60	123.33
1	A	139	MET	N-CA-CB	-5.54	103.47	110.45
1	A	109	VAL	CA-C-O	5.51	126.47	120.57
1	A	108	LYS	CA-C-N	5.50	129.86	122.93
1	A	108	LYS	C-N-CA	5.50	129.86	122.93
1	A	98	LYS	CA-C-N	5.50	128.20	120.28
1	A	98	LYS	C-N-CA	5.50	128.20	120.28
1	A	126	ASN	CB-CA-C	5.47	119.16	109.65
1	A	41	SER	CA-C-O	5.46	126.38	120.43
1	A	87	HIS	CE1-NE2-CD2	5.43	114.43	109.00
1	A	33	TYR	N-CA-C	-5.42	105.28	111.14
1	A	77	ARG	CA-C-N	5.42	133.18	121.64
1	A	77	ARG	C-N-CA	5.42	133.18	121.64
1	A	133	LEU	CA-CB-CG	5.42	135.26	116.30
1	A	100	THR	O-C-N	5.40	128.31	122.15
1	A	35	GLN	CA-C-N	5.40	127.46	120.44
1	A	35	GLN	C-N-CA	5.40	127.46	120.44
1	A	129	GLY	N-CA-C	5.40	118.59	111.52
1	A	146	THR	OG1-CB-CG2	5.38	120.06	109.30
1	A	28	ARG	N-CA-C	5.37	118.04	111.82
1	A	31	GLY	CA-C-O	5.37	126.28	120.75
1	A	172	GLU	CB-CA-C	5.36	120.29	109.68
1	A	42	SER	CA-C-N	5.36	130.51	122.75
1	A	42	SER	C-N-CA	5.36	130.51	122.75
1	A	91	ARG	CG-CD-NE	5.36	123.78	112.00
1	A	71	ILE	N-CA-CB	5.35	117.10	111.00
1	A	152	ASP	N-CA-CB	-5.29	101.47	109.94
1	A	35	GLN	CG-CD-NE2	5.28	124.33	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ASP	CB-CG-OD1	5.28	130.55	118.40
1	A	74	VAL	CA-CB-CG1	5.26	119.35	110.40
1	A	40	THR	N-CA-C	5.24	117.77	109.96
1	A	96	ALA	O-C-N	5.23	127.66	122.12
1	A	74	VAL	O-C-N	-5.22	117.81	123.14
1	A	50	VAL	CB-CA-C	5.21	118.35	110.63
1	A	40	THR	CA-C-O	5.21	126.69	120.70
1	A	30	GLU	N-CA-C	-5.19	105.70	111.36
1	A	122	LYS	CA-C-O	5.17	126.44	120.90
1	A	71	ILE	O-C-N	5.17	129.25	122.94
1	A	128	PRO	CA-C-N	-5.17	113.58	123.03
1	A	128	PRO	C-N-CA	-5.17	113.58	123.03
1	A	143	GLU	CB-CA-C	-5.15	102.90	110.06
1	A	25	PRO	CB-CA-C	5.14	117.19	110.92
1	A	135	VAL	CA-C-O	-5.13	115.06	120.39
1	A	72	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	A	158	LEU	CA-C-O	-5.11	114.66	120.58
1	A	151	ILE	O-C-N	5.10	128.76	122.95
1	A	53	GLY	N-CA-C	-5.10	104.64	112.85
1	A	74	VAL	CA-C-N	5.08	129.74	122.72
1	A	74	VAL	C-N-CA	5.08	129.74	122.72
1	A	89	LEU	CB-CA-C	5.08	118.89	109.70
1	A	134	PHE	N-CA-CB	5.07	118.74	110.37
1	A	2	GLY	CA-C-O	5.06	129.38	120.57
1	A	36	ARG	CA-C-N	5.04	127.29	120.44
1	A	36	ARG	C-N-CA	5.04	127.29	120.44
1	A	30	GLU	CG-CD-OE2	5.03	129.96	118.40
1	A	171	GLU	CA-C-N	-5.02	113.11	121.94
1	A	171	GLU	C-N-CA	-5.02	113.11	121.94
1	A	172	GLU	CG-CD-OE2	-5.01	106.87	118.40

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	1495	0	1504	70	1
2	A	48	0	26	4	0
3	A	32	0	20	0	0
4	A	47	0	0	8	2
All	All	1622	0	1550	71	2

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 (71) 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:55:LYS:HB2	4:A:224:HOH:O	1.54	1.06
1:A:89:LEU:HD13	4:A:234:HOH:O	1.57	1.05
1:A:28:ARG:NE	1:A:32:ARG:NH2	2.11	0.98
1:A:89:LEU:HB2	4:A:234:HOH:O	1.63	0.98
1:A:28:ARG:HE	1:A:32:ARG:CZ	1.78	0.95
1:A:72:ASN:H	1:A:87:HIS:HD2	1.12	0.95
1:A:12:GLN:HB3	1:A:141:ASP:OD1	1.67	0.94
1:A:99:LEU:CD2	1:A:105:LEU:HD12	1.99	0.92
1:A:117:GLY:HA3	2:A:187:NDP:O2A	1.69	0.91
1:A:99:LEU:HD22	1:A:105:LEU:HD12	1.50	0.91
1:A:28:ARG:HE	1:A:32:ARG:NH2	1.67	0.88
1:A:36:ARG:NH1	1:A:37:MET:HE3	1.91	0.84
1:A:129:GLY:O	1:A:184:LYS:NZ	2.10	0.83
1:A:28:ARG:CD	1:A:32:ARG:NH2	2.46	0.79
1:A:28:ARG:NE	1:A:32:ARG:HH22	1.84	0.75
1:A:145:ASP:OD1	1:A:146:THR:HG22	1.86	0.74
1:A:89:LEU:CD1	4:A:234:HOH:O	2.25	0.74
1:A:99:LEU:O	1:A:99:LEU:HD23	1.91	0.71
2:A:187:NDP:H52A	2:A:187:NDP:H8A	1.74	0.70
1:A:36:ARG:NH1	1:A:37:MET:CE	2.55	0.69
1:A:28:ARG:HE	1:A:32:ARG:NH1	1.92	0.68
1:A:72:ASN:H	1:A:87:HIS:CD2	2.04	0.68
1:A:48:ASN:HD21	1:A:111:MET:HE3	1.59	0.67
1:A:121:TYR:O	1:A:125:MET:HB2	1.96	0.66
1:A:48:ASN:ND2	1:A:111:MET:HE3	2.11	0.65
1:A:130:HIS:ND1	1:A:184:LYS:O	2.30	0.64
1:A:26:PRO:O	1:A:173:LYS:HE3	1.98	0.62
1:A:4:LEU:HD12	1:A:112:VAL:HG22	1.82	0.61
1:A:126:ASN:HB2	4:A:216:HOH:O	2.02	0.60
1:A:130:HIS:HE1	1:A:183:GLU:CG	2.15	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:CG	4:A:234:HOH:O	2.51	0.58
1:A:97:LEU:O	1:A:100:THR:HB	2.05	0.57
1:A:99:LEU:HA	1:A:102:GLN:HG2	1.86	0.57
1:A:168:ASP:N	1:A:168:ASP:OD1	2.38	0.56
1:A:111:MET:HE1	4:A:200:HOH:O	2.07	0.55
1:A:99:LEU:HD22	1:A:105:LEU:CD1	2.31	0.54
1:A:107:ASN:ND2	1:A:107:ASN:H	2.04	0.54
1:A:10:VAL:HG22	1:A:14:MET:HA	1.90	0.54
1:A:37:MET:HA	1:A:37:MET:HE2	1.89	0.54
1:A:159:LEU:HD12	1:A:181:VAL:HG22	1.89	0.53
1:A:4:LEU:HD11	1:A:114:ILE:HD11	1.91	0.53
1:A:156:TYR:CZ	1:A:184:LYS:HD3	2.43	0.53
1:A:168:ASP:O	1:A:170:GLN:NE2	2.36	0.52
1:A:4:LEU:HD11	1:A:114:ILE:CD1	2.40	0.52
1:A:152:ASP:OD2	1:A:155:LYS:HE2	2.11	0.51
1:A:100:THR:HG22	1:A:101:GLU:N	2.26	0.51
1:A:28:ARG:NE	1:A:32:ARG:CZ	2.56	0.50
1:A:156:TYR:OH	1:A:184:LYS:HD3	2.11	0.50
1:A:114:ILE:HD13	1:A:124:ALA:HB2	1.93	0.50
1:A:117:GLY:HA3	2:A:187:NDP:PA	2.52	0.49
1:A:16:ILE:O	2:A:187:NDP:H2N	2.13	0.48
1:A:99:LEU:CD2	1:A:105:LEU:CD1	2.82	0.48
1:A:130:HIS:CE1	1:A:183:GLU:CG	2.96	0.47
1:A:36:ARG:CZ	1:A:37:MET:HE3	2.44	0.46
1:A:114:ILE:HD13	1:A:124:ALA:CB	2.45	0.45
1:A:28:ARG:HD2	1:A:32:ARG:NH2	2.28	0.44
1:A:99:LEU:HD23	1:A:99:LEU:C	2.42	0.44
1:A:95:ASP:OD1	1:A:98:LYS:NZ	2.39	0.44
1:A:80:LYS:HB3	1:A:80:LYS:HE3	1.71	0.43
1:A:130:HIS:HD1	1:A:185:ASN:HB2	1.84	0.43
1:A:24:TRP:HB2	1:A:25:PRO:HD2	2.01	0.43
1:A:43:VAL:HG11	1:A:46:LYS:HD2	2.00	0.43
1:A:130:HIS:CE1	1:A:183:GLU:HG3	2.54	0.42
1:A:172:GLU:C	1:A:174:GLY:N	2.76	0.42
1:A:42:SER:OG	1:A:110:ASP:OD2	2.30	0.42
1:A:89:LEU:CB	4:A:234:HOH:O	2.35	0.42
1:A:186:ASP:OD1	1:A:186:ASP:O	2.37	0.41
1:A:114:ILE:HG23	1:A:120:VAL:HG12	2.03	0.41
1:A:140:GLN:HG3	1:A:142:PHE:CE2	2.56	0.40
1:A:145:ASP:OD1	1:A:146:THR:CG2	2.65	0.40
1:A:186:ASP:OD1	1:A:186:ASP:C	2.64	0.40

All (2) 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)
4:A:192:HOH:O	4:A:229:HOH:O[8_544]	2.06	0.14
1:A:154:GLU:OE1	4:A:204:HOH:O[8_544]	2.11	0.09

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	184/186 (99%)	178 (97%)	5 (3%)	1 (0%)	24 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	GLU

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	167/167 (100%)	144 (86%)	23 (14%)	3 2

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

Mol	Chain	Res	Type
1	A	3	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	18	LYS
1	A	22	LEU
1	A	28	ARG
1	A	65	ARG
1	A	66	PRO
1	A	68	LYS
1	A	72	ASN
1	A	89	LEU
1	A	100	THR
1	A	104	GLU
1	A	107	ASN
1	A	112	VAL
1	A	118	SER
1	A	119	SER
1	A	123	GLU
1	A	125	MET
1	A	133	LEU
1	A	146	THR
1	A	150	GLU
1	A	168	ASP
1	A	178	LYS
1	A	181	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	48	ASN
1	A	87	HIS
1	A	127	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	NDP	A	187	-	51,52,52	2.56	18 (35%)	71,80,80	2.25	24 (33%)
3	MOT	A	188	-	34,34,34	3.31	13 (38%)	41,48,48	3.69	24 (58%)

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	187	-	-	11/34/77/77	0/5/5/5
3	MOT	A	188	-	-	3/25/25/25	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	188	MOT	C4A-C4	-10.81	1.30	1.42
2	A	187	NDP	O4B-C4B	-8.77	1.25	1.45
2	A	187	NDP	P2B-O2B	7.82	1.73	1.59
3	A	188	MOT	O8-C8A	-7.18	1.27	1.37
3	A	188	MOT	C11-C	-6.18	1.36	1.50
3	A	188	MOT	O8-C7	-5.85	1.21	1.38
2	A	187	NDP	C5A-C6A	5.31	1.55	1.41
3	A	188	MOT	C4A-C8A	-4.85	1.34	1.39
3	A	188	MOT	C4-N3	-4.75	1.28	1.35
2	A	187	NDP	O4D-C1D	4.02	1.51	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	C5A-C4A	-3.97	1.32	1.39
2	A	187	NDP	C3B-C4B	3.95	1.63	1.53
3	A	188	MOT	C2-N3	-3.77	1.28	1.35
2	A	187	NDP	O3B-C3B	3.31	1.51	1.43
3	A	188	MOT	C9-N10	3.21	1.51	1.46
3	A	188	MOT	C16-C15	-3.05	1.33	1.38
2	A	187	NDP	C1D-N1N	2.82	1.54	1.46
2	A	187	NDP	PN-O2N	-2.82	1.42	1.55
2	A	187	NDP	PA-O2A	-2.74	1.42	1.55
2	A	187	NDP	O2B-C2B	-2.73	1.34	1.44
2	A	187	NDP	C5A-N7A	2.73	1.44	1.39
3	A	188	MOT	C2-N1	-2.71	1.30	1.35
2	A	187	NDP	C3D-C4D	2.55	1.59	1.53
3	A	188	MOT	O2-CT	-2.49	1.22	1.30
3	A	188	MOT	OE2-CD	-2.45	1.22	1.30
2	A	187	NDP	C4A-N3A	2.43	1.39	1.34
2	A	187	NDP	C4N-C3N	2.41	1.54	1.50
2	A	187	NDP	C4A-N9A	-2.38	1.32	1.37
2	A	187	NDP	C2B-C1B	2.11	1.58	1.53
3	A	188	MOT	CB-CA	2.06	1.58	1.53
2	A	187	NDP	PA-O5B	2.01	1.67	1.59

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188	MOT	O8-C8A-N1	10.16	124.60	119.20
3	A	188	MOT	NA2-C2-N3	7.90	129.07	117.22
3	A	188	MOT	CB-CA-CT	-6.72	94.42	110.35
3	A	188	MOT	O8-C8A-C4A	6.23	114.02	110.00
3	A	188	MOT	CA-N-C	5.85	135.60	121.56
3	A	188	MOT	C2-N3-C4	5.57	123.97	117.28
3	A	188	MOT	CM-N10-C14	5.43	128.58	119.59
2	A	187	NDP	O7N-C7N-C3N	-5.04	111.40	120.90
2	A	187	NDP	PN-O5D-C5D	4.91	149.50	121.35
3	A	188	MOT	C16-C15-C14	4.34	125.79	120.30
3	A	188	MOT	NA2-C2-N1	-4.33	110.73	117.22
2	A	187	NDP	O3-PA-O1A	-4.30	97.78	110.70
3	A	188	MOT	C8A-O8-C7	4.27	108.53	105.80
3	A	188	MOT	C16-C11-C12	-4.24	113.17	118.57
2	A	187	NDP	O4D-C1D-N1N	-4.23	100.02	108.08
2	A	187	NDP	C6N-N1N-C2N	4.16	123.77	119.32
2	A	187	NDP	C2D-C1D-N1N	4.15	123.51	113.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	187	NDP	C3N-C2N-N1N	-4.03	117.28	123.20
2	A	187	NDP	C3N-C7N-N7N	4.03	124.83	117.67
3	A	188	MOT	O1-CT-CA	-3.96	109.50	122.26
2	A	187	NDP	C4B-O4B-C1B	3.80	117.85	109.47
2	A	187	NDP	O3D-C3D-C4D	-3.66	100.56	111.08
2	A	187	NDP	C5A-C4A-N9A	3.62	109.76	105.81
3	A	188	MOT	C13-C14-N10	3.57	126.57	121.59
2	A	187	NDP	O4B-C1B-N9A	3.50	114.81	108.09
3	A	188	MOT	N3-C2-N1	-3.45	120.19	125.48
2	A	187	NDP	O4B-C1B-C2B	-3.43	100.68	106.59
2	A	187	NDP	O3D-C3D-C2D	3.39	122.69	111.82
3	A	188	MOT	OE1-CD-CG	-3.26	112.74	123.09
2	A	187	NDP	O3-PN-O1N	3.25	120.49	110.70
3	A	188	MOT	C15-C14-C13	-3.20	113.08	119.18
2	A	187	NDP	O3B-C3B-C4B	-2.93	102.67	111.08
2	A	187	NDP	O2A-PA-O1A	2.88	125.85	112.44
3	A	188	MOT	C13-C12-C11	2.84	123.83	120.80
2	A	187	NDP	O5B-C5B-C4B	-2.83	99.36	108.99
2	A	187	NDP	C1D-N1N-C2N	-2.79	116.55	121.14
3	A	188	MOT	CB-CA-N	2.72	116.28	110.91
3	A	188	MOT	O2-CT-O1	2.64	130.08	124.08
2	A	187	NDP	C5B-C4B-C3B	-2.60	105.86	115.21
2	A	187	NDP	O5D-C5D-C4D	-2.49	100.52	108.99
3	A	188	MOT	CM-N10-C9	-2.38	108.56	114.49
2	A	187	NDP	C6A-C5A-N7A	2.37	136.66	132.09
3	A	188	MOT	O-C-N	-2.37	117.96	122.47
3	A	188	MOT	C4A-C4-NA4	2.31	126.46	123.40
3	A	188	MOT	OE2-CD-OE1	2.23	129.06	123.33
3	A	188	MOT	C9-C6-C4A	2.16	129.57	126.26
2	A	187	NDP	C2B-C3B-C4B	-2.10	97.49	101.99
2	A	187	NDP	O3X-P2B-O1X	2.01	118.66	110.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	187	NDP	C5D-O5D-PN-O1N
2	A	187	NDP	C5D-O5D-PN-O2N
2	A	187	NDP	C3D-C4D-C5D-O5D
2	A	187	NDP	O4D-C4D-C5D-O5D
2	A	187	NDP	C5D-O5D-PN-O3
2	A	187	NDP	C2B-O2B-P2B-O3X

Continued on next page...

Continued from previous page...

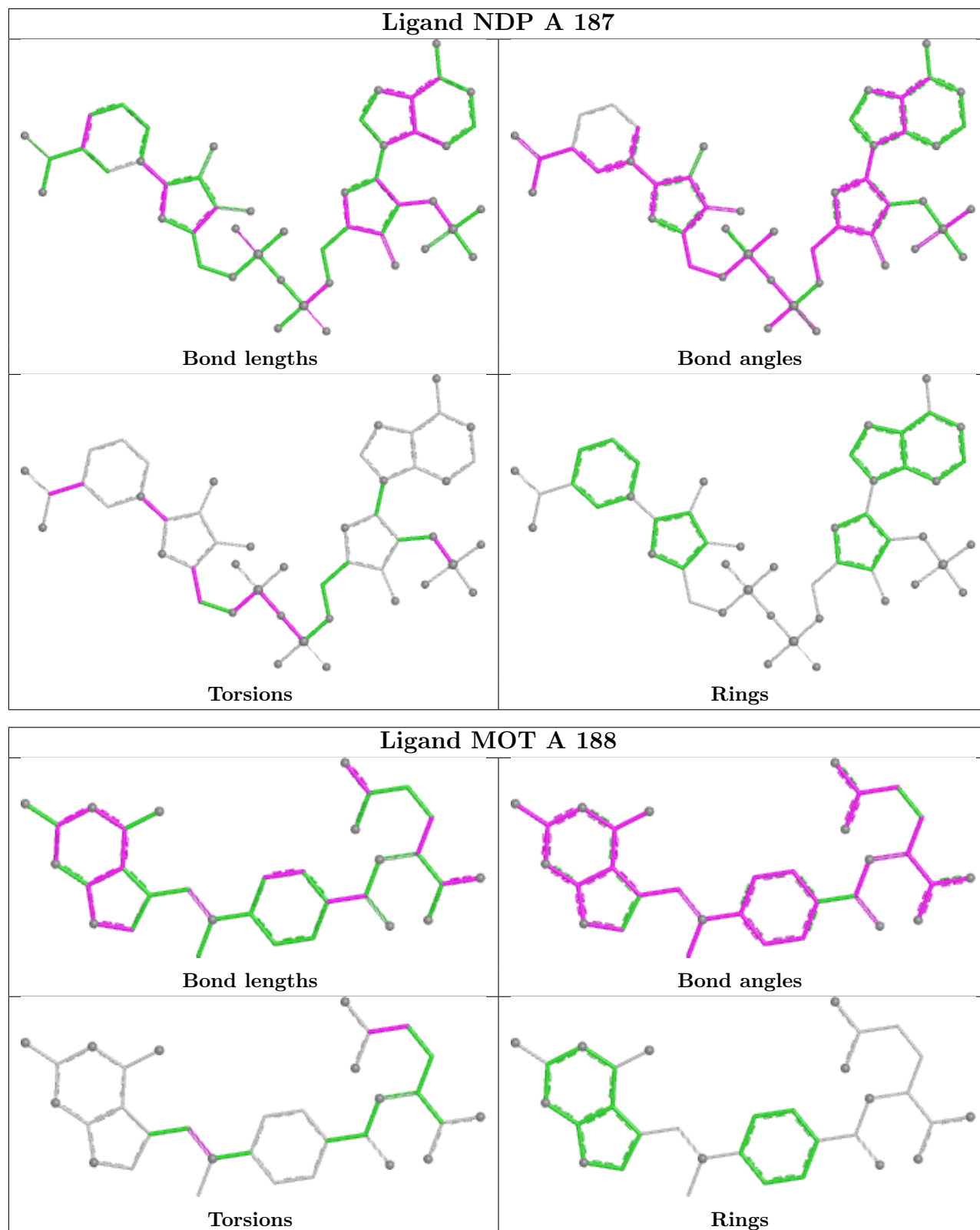
Mol	Chain	Res	Type	Atoms
2	A	187	NDP	O4D-C1D-N1N-C2N
2	A	187	NDP	C2N-C3N-C7N-N7N
3	A	188	MOT	OE1-CD-CG-CB
3	A	188	MOT	OE2-CD-CG-CB
2	A	187	NDP	C2D-C1D-N1N-C2N
2	A	187	NDP	PN-O3-PA-O1A
2	A	187	NDP	PA-O3-PN-O2N
3	A	188	MOT	C6-C9-N10-CM

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	187	NDP	4	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.