



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:11 am BST

PDB ID : 1HFR  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

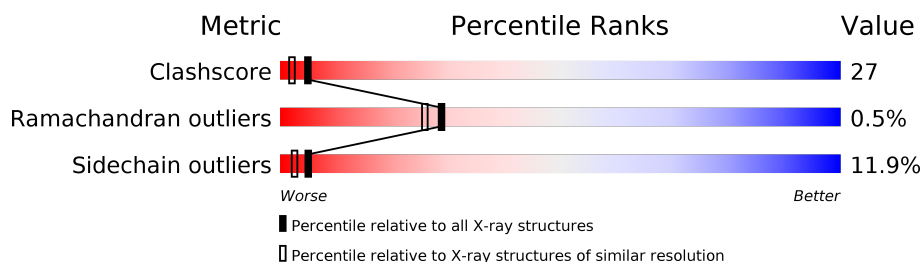
# 1 Overall quality at a glance

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)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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](#)

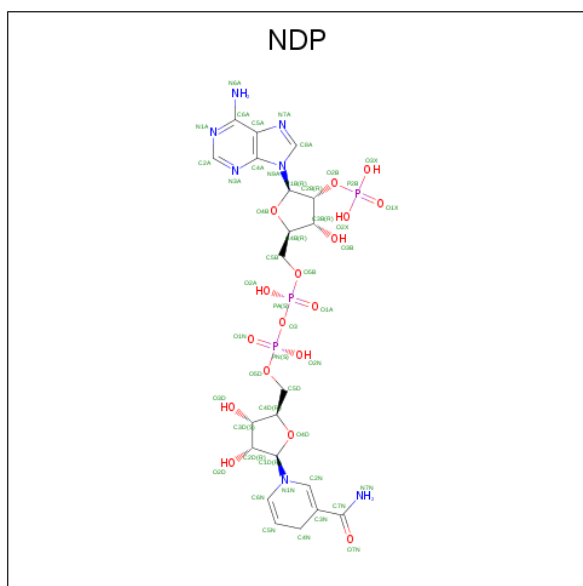
There are 4 unique types of molecules in this entry. The entry contains 1617 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

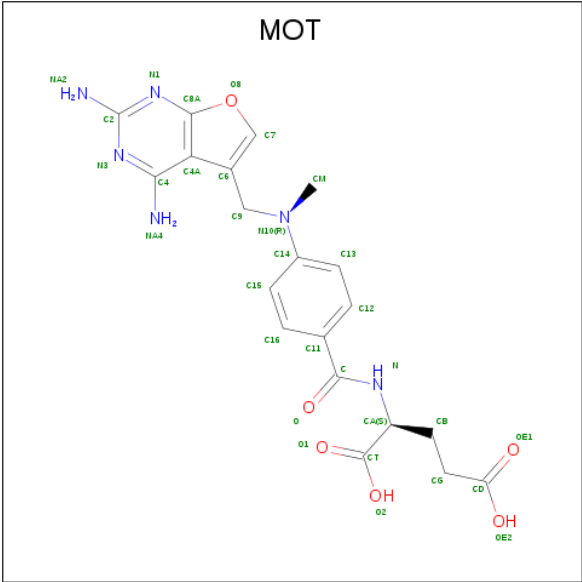
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1502	963	253	279	7	0	0	0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: 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 (three-letter code: 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.

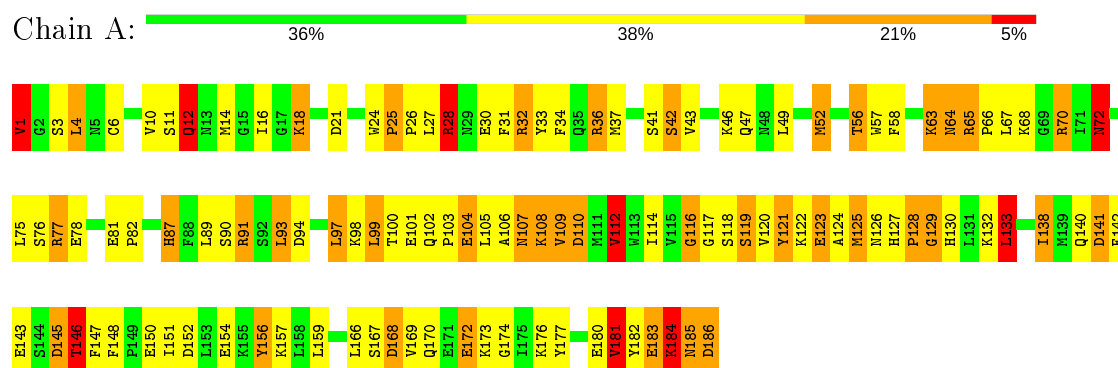
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.90 Å 86.90 Å 77.09 Å 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
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, $R_{free}$	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1617	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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: NDP, MOT

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	1.39	5/1537 (0.3%)	2.71	122/2073 (5.9%)

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	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	GLU	CG-CD	-7.54	1.40	1.51
1	A	172	GLU	CD-OE2	-7.29	1.17	1.25
1	A	67	LEU	N-CA	5.26	1.56	1.46
1	A	154	GLU	CG-CD	-5.14	1.44	1.51
1	A	119	SER	CB-OG	5.10	1.48	1.42

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ASP	CB-CG-OD2	17.78	134.30	118.30
1	A	70	ARG	NE-CZ-NH2	-15.90	112.35	120.30
1	A	141	ASP	CB-CG-OD1	-14.97	104.83	118.30
1	A	77	ARG	NE-CZ-NH1	-14.53	113.04	120.30
1	A	77	ARG	CD-NE-CZ	-11.43	107.60	123.60
1	A	1	VAL	CA-CB-CG1	11.21	127.72	110.90
1	A	21	ASP	CB-CG-OD2	-10.97	108.42	118.30
1	A	116	GLY	C-N-CA	10.71	144.80	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ARG	NH1-CZ-NH2	10.35	130.79	119.40
1	A	141	ASP	CB-CG-OD2	10.05	127.34	118.30
1	A	154	GLU	OE1-CD-OE2	-9.78	111.56	123.30
1	A	77	ARG	NE-CZ-NH2	-9.74	115.43	120.30
1	A	123	GLU	OE1-CD-OE2	9.73	134.98	123.30
1	A	141	ASP	CA-CB-CG	-9.65	92.16	113.40
1	A	28	ARG	NE-CZ-NH2	9.62	125.11	120.30
1	A	146	THR	CA-CB-CG2	9.31	125.43	112.40
1	A	181	VAL	CA-CB-CG2	9.03	124.45	110.90
1	A	65	ARG	CD-NE-CZ	9.01	136.22	123.60
1	A	1	VAL	CB-CA-C	8.73	127.98	111.40
1	A	145	ASP	CB-CG-OD1	8.52	125.97	118.30
1	A	91	ARG	NE-CZ-NH1	-8.48	116.06	120.30
1	A	91	ARG	CD-NE-CZ	-8.22	112.09	123.60
1	A	110	ASP	OD1-CG-OD2	-8.20	107.72	123.30
1	A	70	ARG	NH1-CZ-NH2	8.19	128.41	119.40
1	A	21	ASP	CB-CG-OD1	8.05	125.55	118.30
1	A	36	ARG	NE-CZ-NH2	8.05	124.32	120.30
1	A	112	VAL	CG1-CB-CG2	8.04	123.76	110.90
1	A	182	TYR	CB-CG-CD2	-7.99	116.21	121.00
1	A	169	VAL	CA-CB-CG2	7.91	122.77	110.90
1	A	186	ASP	CA-C-O	-7.78	103.77	120.10
1	A	4	LEU	CB-CG-CD2	-7.68	97.95	111.00
1	A	133	LEU	CA-CB-CG	7.64	132.87	115.30
1	A	77	ARG	CA-CB-CG	-7.58	96.73	113.40
1	A	30	GLU	OE1-CD-OE2	-7.57	114.22	123.30
1	A	32	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	A	154	GLU	CG-CD-OE1	7.51	133.32	118.30
1	A	91	ARG	CA-CB-CG	-7.50	96.89	113.40
1	A	147	PHE	CG-CD1-CE1	7.42	128.97	120.80
1	A	78	GLU	CA-CB-CG	7.35	129.56	113.40
1	A	72	ASN	O-C-N	7.33	134.43	122.70
1	A	133	LEU	CB-CG-CD1	7.30	123.42	111.00
1	A	110	ASP	CB-CA-C	7.29	124.98	110.40
1	A	91	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	180	GLU	CG-CD-OE2	7.21	132.72	118.30
1	A	91	ARG	NH1-CZ-NH2	7.16	127.28	119.40
1	A	56	THR	CA-CB-OG1	-7.13	94.03	109.00
1	A	180	GLU	OE1-CD-OE2	-7.11	114.77	123.30
1	A	33	TYR	CB-CG-CD2	7.06	125.23	121.00
1	A	97	LEU	CB-CG-CD2	-6.98	99.14	111.00
1	A	168	ASP	CB-CG-OD1	-6.90	112.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	SER	N-CA-CB	6.87	120.80	110.50
1	A	126	ASN	CA-CB-CG	6.77	128.30	113.40
1	A	66	PRO	N-CD-CG	-6.72	93.11	103.20
1	A	11	SER	O-C-N	-6.70	111.98	122.70
1	A	110	ASP	O-C-N	-6.66	112.05	122.70
1	A	58	PHE	CB-CG-CD2	-6.64	116.15	120.80
1	A	168	ASP	CA-CB-CG	-6.59	98.91	113.40
1	A	112	VAL	CA-CB-CG2	-6.54	101.09	110.90
1	A	125	MET	CA-CB-CG	-6.53	102.19	113.30
1	A	154	GLU	CB-CG-CD	6.53	131.83	114.20
1	A	25	PRO	CB-CA-C	6.35	127.88	112.00
1	A	183	GLU	OE1-CD-OE2	6.31	130.87	123.30
1	A	49	LEU	CB-CG-CD1	-6.22	100.43	111.00
1	A	177	TYR	O-C-N	6.20	132.61	122.70
1	A	12	GLN	CG-CD-OE1	-6.18	109.24	121.60
1	A	93	LEU	CB-CG-CD2	-6.18	100.49	111.00
1	A	112	VAL	CA-CB-CG1	6.12	120.08	110.90
1	A	58	PHE	CD1-CG-CD2	6.11	126.24	118.30
1	A	58	PHE	CD1-CE1-CZ	-6.11	112.77	120.10
1	A	72	ASN	CA-C-O	-6.10	107.30	120.10
1	A	77	ARG	CG-CD-NE	-6.05	99.09	111.80
1	A	101	GLU	CB-CG-CD	6.03	130.48	114.20
1	A	32	ARG	CA-CB-CG	-6.01	100.17	113.40
1	A	184	LYS	CD-CE-NZ	-6.01	97.87	111.70
1	A	181	VAL	CA-CB-CG1	5.94	119.82	110.90
1	A	42	SER	CA-C-O	-5.91	107.68	120.10
1	A	129	GLY	O-C-N	5.90	132.14	122.70
1	A	150	GLU	CG-CD-OE1	-5.90	106.50	118.30
1	A	101	GLU	CB-CA-C	-5.88	98.65	110.40
1	A	122	LYS	CD-CE-NZ	-5.83	98.28	111.70
1	A	147	PHE	CD1-CE1-CZ	-5.83	113.11	120.10
1	A	87	HIS	CG-ND1-CE1	5.81	116.33	108.20
1	A	57	TRP	O-C-N	-5.77	113.47	122.70
1	A	108	LYS	N-CA-CB	-5.76	100.22	110.60
1	A	132	LYS	CD-CE-NZ	-5.74	98.49	111.70
1	A	128	PRO	C-N-CA	-5.71	110.30	122.30
1	A	30	GLU	CB-CA-C	5.70	121.80	110.40
1	A	126	ASN	CB-CG-OD1	5.68	132.96	121.60
1	A	176	LYS	O-C-N	5.64	131.72	122.70
1	A	31	PHE	N-CA-CB	5.62	120.72	110.60
1	A	30	GLU	O-C-N	-5.58	113.78	122.70
1	A	152	ASP	N-CA-CB	-5.54	100.62	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	LYS	CA-CB-CG	-5.54	101.22	113.40
1	A	6	CYS	N-CA-CB	5.53	120.56	110.60
1	A	138	ILE	N-CA-C	-5.51	96.12	111.00
1	A	176	LYS	CD-CE-NZ	-5.47	99.12	111.70
1	A	185	ASN	N-CA-CB	5.46	120.44	110.60
1	A	91	ARG	O-C-N	5.44	131.40	122.70
1	A	99	LEU	CA-CB-CG	5.41	127.73	115.30
1	A	172	GLU	CA-CB-CG	5.40	125.29	113.40
1	A	58	PHE	CG-CD2-CE2	-5.39	114.87	120.80
1	A	3	SER	O-C-N	5.37	131.29	122.70
1	A	157	LYS	CA-CB-CG	-5.37	101.60	113.40
1	A	145	ASP	CB-CA-C	5.36	121.13	110.40
1	A	42	SER	CB-CA-C	-5.34	99.96	110.10
1	A	156	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	168	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	11	SER	CA-C-O	5.24	131.11	120.10
1	A	108	LYS	N-CA-C	5.24	125.15	111.00
1	A	122	LYS	CA-CB-CG	-5.19	101.98	113.40
1	A	123	GLU	CG-CD-OE1	-5.18	107.95	118.30
1	A	18	LYS	CA-CB-CG	-5.17	102.02	113.40
1	A	41	SER	CA-CB-OG	-5.14	97.31	111.20
1	A	18	LYS	CD-CE-NZ	-5.13	99.90	111.70
1	A	109	VAL	CA-CB-CG1	5.13	118.59	110.90
1	A	183	GLU	CG-CD-OE1	-5.11	108.08	118.30
1	A	33	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	A	143	GLU	CB-CA-C	-5.07	100.26	110.40
1	A	64	ASN	CA-C-O	-5.05	109.49	120.10
1	A	27	LEU	CB-CG-CD2	5.05	119.59	111.00
1	A	121	TYR	CD1-CE1-CZ	-5.04	115.27	119.80
1	A	91	ARG	CG-CD-NE	-5.01	101.28	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	MET	Mainchain
1	A	77	ARG	Sidechain

## 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	1502	0	1510	86	0
2	A	48	0	26	3	0
3	A	32	0	20	1	0
4	A	35	0	0	4	0
All	All	1617	0	1556	86	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 27.

All (86) 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:1:VAL:HG12	1:A:109:VAL:O	1.36	1.23
1:A:1:VAL:CG1	1:A:109:VAL:O	2.02	1.06
1:A:145:ASP:OD1	1:A:146:THR:HG22	1.56	1.04
1:A:99:LEU:HD22	1:A:105:LEU:HD12	1.50	0.93
1:A:28:ARG:HE	1:A:32:ARG:HH22	1.13	0.91
1:A:28:ARG:HE	1:A:32:ARG:NH2	1.68	0.90
1:A:72:ASN:H	1:A:87:HIS:HD2	1.21	0.86
1:A:116:GLY:HA2	1:A:121:TYR:CE2	2.10	0.86
1:A:99:LEU:CD2	1:A:105:LEU:HD12	2.06	0.85
1:A:107:ASN:ND2	1:A:107:ASN:H	1.74	0.84
1:A:28:ARG:NE	1:A:32:ARG:NH2	2.31	0.78
1:A:168:ASP:OD1	1:A:168:ASP:N	2.17	0.76
1:A:98:LYS:NZ	4:A:207:HOH:O	2.18	0.75
1:A:93:LEU:CD2	1:A:123:GLU:HG2	2.18	0.73
1:A:129:GLY:O	1:A:184:LYS:NZ	2.21	0.73
1:A:93:LEU:HD22	1:A:123:GLU:HG2	1.70	0.72
1:A:72:ASN:H	1:A:87:HIS:CD2	2.09	0.68
1:A:166:LEU:N	1:A:166:LEU:HD12	2.09	0.68
1:A:114:ILE:HD13	1:A:124:ALA:HB2	1.75	0.68
1:A:166:LEU:CD1	1:A:166:LEU:N	2.58	0.66
1:A:116:GLY:HA3	2:A:187:NDP:H5N	1.78	0.63
1:A:99:LEU:HD22	1:A:105:LEU:CD1	2.28	0.62
1:A:141:ASP:N	1:A:141:ASP:OD1	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:CG2	1:A:14:MET:HA	2.29	0.61
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.83	0.61
1:A:130:HIS:ND1	1:A:184:LYS:O	2.31	0.60
1:A:168:ASP:O	1:A:170:GLN:NE2	2.30	0.59
1:A:130:HIS:HE1	1:A:183:GLU:CG	2.15	0.59
1:A:156:TYR:CZ	1:A:184:LYS:HD3	2.37	0.59
1:A:99:LEU:HD23	1:A:99:LEU:O	2.03	0.59
1:A:123:GLU:OE1	2:A:187:NDP:N6A	2.37	0.58
1:A:186:ASP:OD1	1:A:186:ASP:C	2.41	0.58
1:A:1:VAL:HG21	1:A:106:ALA:O	2.04	0.58
1:A:114:ILE:HD13	1:A:124:ALA:CB	2.34	0.58
1:A:47:GLN:O	1:A:109:VAL:HA	2.04	0.58
1:A:159:LEU:HD12	1:A:181:VAL:HG22	1.85	0.57
1:A:1:VAL:HG11	1:A:109:VAL:O	2.01	0.57
1:A:107:ASN:N	1:A:107:ASN:ND2	2.38	0.56
1:A:36:ARG:NH1	1:A:37:MET:HE1	2.20	0.56
1:A:166:LEU:CD1	1:A:166:LEU:H	2.18	0.56
1:A:42:SER:N	1:A:110:ASP:OD2	2.30	0.56
1:A:36:ARG:NH1	1:A:37:MET:CE	2.68	0.56
1:A:93:LEU:O	1:A:97:LEU:HG	2.05	0.56
1:A:117:GLY:O	1:A:121:TYR:CD2	2.59	0.55
1:A:36:ARG:HH12	1:A:37:MET:HE1	1.73	0.54
1:A:94:ASP:HB2	4:A:207:HOH:O	2.08	0.54
1:A:42:SER:OG	1:A:110:ASP:OD2	2.21	0.54
1:A:102:GLN:HB3	1:A:104:GLU:HG3	1.90	0.53
1:A:26:PRO:O	1:A:173:LYS:HE3	2.08	0.53
1:A:103:PRO:O	1:A:104:GLU:C	2.46	0.53
1:A:117:GLY:O	1:A:121:TYR:HD2	1.91	0.52
1:A:63:LYS:HG2	1:A:64:ASN:N	2.21	0.52
1:A:127:HIS:HD2	4:A:206:HOH:O	1.93	0.52
1:A:43:VAL:HG11	1:A:46:LYS:HE3	1.91	0.51
1:A:99:LEU:CD2	1:A:105:LEU:CD1	2.84	0.51
1:A:28:ARG:NE	1:A:32:ARG:HH22	1.92	0.50
1:A:99:LEU:HA	1:A:102:GLN:HG2	1.92	0.50
1:A:93:LEU:HD23	1:A:123:GLU:HG2	1.93	0.48
1:A:114:ILE:HG23	1:A:120:VAL:HG12	1.94	0.48
1:A:16:ILE:O	2:A:187:NDP:H2N	2.13	0.48
1:A:145:ASP:OD1	1:A:146:THR:CG2	2.45	0.47
1:A:140:GLN:C	1:A:141:ASP:OD1	2.53	0.47
1:A:91:ARG:HD2	4:A:215:HOH:O	2.16	0.45
1:A:4:LEU:HD12	1:A:112:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLU:C	1:A:174:GLY:N	2.71	0.45
1:A:166:LEU:HD13	1:A:166:LEU:H	1.82	0.45
1:A:24:TRP:CB	1:A:25:PRO:HD2	2.47	0.44
1:A:130:HIS:CE1	1:A:183:GLU:OE2	2.70	0.44
1:A:107:ASN:C	1:A:107:ASN:HD22	2.20	0.44
1:A:93:LEU:HD23	1:A:123:GLU:CG	2.48	0.43
1:A:70:ARG:NH2	3:A:188:MOT:O2	2.25	0.43
1:A:81:GLU:HB2	1:A:82:PRO:HD2	2.00	0.42
1:A:28:ARG:O	1:A:32:ARG:HG3	2.20	0.42
1:A:125:MET:HG2	1:A:133:LEU:HD11	2.01	0.42
1:A:121:TYR:CD1	1:A:148:PHE:HE1	2.38	0.42
1:A:151:ILE:HD13	1:A:151:ILE:HG21	1.88	0.41
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.76	0.41
1:A:24:TRP:HB3	1:A:142:PHE:CZ	2.55	0.41
1:A:34:PHE:C	1:A:34:PHE:CD1	2.93	0.41
1:A:156:TYR:CD1	1:A:184:LYS:HB2	2.56	0.41
1:A:76:SER:HB3	1:A:89:LEU:HD11	2.01	0.41
1:A:108:LYS:HE2	1:A:108:LYS:HB2	1.80	0.41
1:A:12:GLN:HB3	1:A:141:ASP:OD1	2.21	0.41
1:A:52:MET:HB2	1:A:56:THR:HB	2.02	0.41
1:A:127:HIS:CG	1:A:128:PRO:HD2	2.57	0.40
1:A:124:ALA:O	1:A:127:HIS:HB3	2.21	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	184/186 (99%)	177 (96%)	6 (3%)	1 (0%)	29	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	168/168 (100%)	148 (88%)	20 (12%)	<b>5</b> <b>2</b>

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	12	GLN
1	A	18	LYS
1	A	28	ARG
1	A	63	LYS
1	A	65	ARG
1	A	68	LYS
1	A	72	ASN
1	A	100	THR
1	A	107	ASN
1	A	112	VAL
1	A	118	SER
1	A	119	SER
1	A	133	LEU
1	A	138	ILE
1	A	146	THR
1	A	167	SER
1	A	181	VAL
1	A	184	LYS
1	A	185	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN

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Mol	Chain	Res	Type
1	A	87	HIS
1	A	107	ASN
1	A	127	HIS
1	A	185	ASN

### 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 carbohydrates 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	MOT	A	188	-	25,34,34	2.33	7 (28%)	28,48,48	3.12	16 (57%)
2	NDP	A	187	-	45,52,52	2.84	19 (42%)	53,80,80	2.50	21 (39%)

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	MOT	A	188	-	-	2/18/25/25	0/3/3/3
2	NDP	A	187	-	-	11/30/77/77	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	P2B-O2B	8.79	1.75	1.59
2	A	187	NDP	O4B-C4B	-8.67	1.25	1.45
3	A	188	MOT	C11-C	-6.03	1.37	1.50
2	A	187	NDP	O4D-C1D	5.07	1.54	1.42
3	A	188	MOT	C2-N3	-4.48	1.27	1.35
2	A	187	NDP	C3B-C4B	4.35	1.64	1.53
2	A	187	NDP	O3B-C3B	4.26	1.53	1.43
3	A	188	MOT	CB-CA	4.11	1.58	1.53
2	A	187	NDP	C5A-C4A	-4.07	1.30	1.40
2	A	187	NDP	C6A-C5A	3.77	1.57	1.43
2	A	187	NDP	C1D-N1N	3.48	1.56	1.46
3	A	188	MOT	C15-C14	-3.48	1.32	1.39
3	A	188	MOT	C4-N3	-3.39	1.27	1.33
2	A	187	NDP	PN-O1N	-3.33	1.39	1.50
2	A	187	NDP	C3D-C4D	3.09	1.60	1.53
3	A	188	MOT	C4A-C8A	-3.08	1.34	1.42
2	A	187	NDP	C8A-N7A	-2.91	1.29	1.34
2	A	187	NDP	PA-O1A	-2.87	1.40	1.50
2	A	187	NDP	P2B-O3X	-2.85	1.43	1.54
2	A	187	NDP	C6A-N1A	-2.85	1.24	1.37
2	A	187	NDP	PN-O2N	-2.61	1.43	1.55
3	A	188	MOT	C16-C15	-2.48	1.34	1.38
2	A	187	NDP	PN-O5D	2.21	1.68	1.59
2	A	187	NDP	O7N-C7N	-2.19	1.19	1.24
2	A	187	NDP	C5B-C4B	2.10	1.58	1.51
2	A	187	NDP	C4A-N3A	2.06	1.38	1.35

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188	MOT	CB-CA-N	-5.88	101.64	110.19
2	A	187	NDP	PN-O3-PA	5.81	152.75	132.83
2	A	187	NDP	O4D-C1D-N1N	-5.65	97.01	108.06
2	A	187	NDP	C3N-C2N-N1N	-5.26	115.59	123.10
3	A	188	MOT	O-C-N	-5.19	112.90	122.45
3	A	188	MOT	C4A-C4-NA4	5.09	131.86	122.67
2	A	187	NDP	O3D-C3D-C4D	-5.07	96.38	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	187	NDP	O4B-C1B-C2B	-4.90	98.08	106.59
2	A	187	NDP	C5B-C4B-C3B	-4.43	98.59	115.18
3	A	188	MOT	C16-C15-C14	4.38	126.08	120.32
2	A	187	NDP	O3B-C3B-C4B	-4.35	98.46	111.05
3	A	188	MOT	N1-C2-N3	-4.29	121.50	127.22
3	A	188	MOT	CB-CG-CD	-4.08	104.83	113.59
3	A	188	MOT	CA-N-C	4.03	127.53	122.34
3	A	188	MOT	CM-N10-C9	-3.89	104.52	114.84
3	A	188	MOT	NA2-C2-N3	3.85	123.25	117.25
3	A	188	MOT	CM-N10-C14	3.74	126.04	119.57
2	A	187	NDP	PN-O5D-C5D	3.70	143.38	121.68
2	A	187	NDP	C1B-N9A-C4A	3.69	133.13	126.64
3	A	188	MOT	C2-N3-C4	3.50	126.71	116.72
3	A	188	MOT	C16-C11-C12	-3.34	113.82	118.59
3	A	188	MOT	O-C-C11	3.22	126.69	120.94
2	A	187	NDP	O2X-P2B-O2B	-3.07	92.25	105.99
2	A	187	NDP	O4D-C4D-C5D	2.94	119.05	109.37
2	A	187	NDP	O3X-P2B-O1X	2.89	122.00	110.68
2	A	187	NDP	O2N-PN-O5D	-2.78	94.86	107.75
2	A	187	NDP	C5A-C6A-N6A	-2.68	116.29	120.35
2	A	187	NDP	O5B-C5B-C4B	-2.67	99.80	108.99
3	A	188	MOT	C13-C12-C11	2.59	123.80	120.78
2	A	187	NDP	N6A-C6A-N1A	2.54	123.85	118.57
2	A	187	NDP	O5D-C5D-C4D	-2.53	100.27	108.99
3	A	188	MOT	C4A-C4-N3	-2.45	116.35	122.73
2	A	187	NDP	O4B-C4B-C3B	-2.44	100.29	105.11
2	A	187	NDP	O7N-C7N-C3N	-2.34	116.50	120.90
2	A	187	NDP	C2B-C3B-C4B	-2.26	97.09	101.99
3	A	188	MOT	C15-C14-C13	-2.17	114.73	119.16
2	A	187	NDP	C2D-C1D-N1N	2.04	118.42	113.30

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	187	NDP	C5D-O5D-PN-O3
2	A	187	NDP	C5D-O5D-PN-O2N
2	A	187	NDP	C3D-C4D-C5D-O5D
3	A	188	MOT	CT-CA-N-C
2	A	187	NDP	C5B-O5B-PA-O3
2	A	187	NDP	C2B-O2B-P2B-O3X
2	A	187	NDP	PA-O3-PN-O1N

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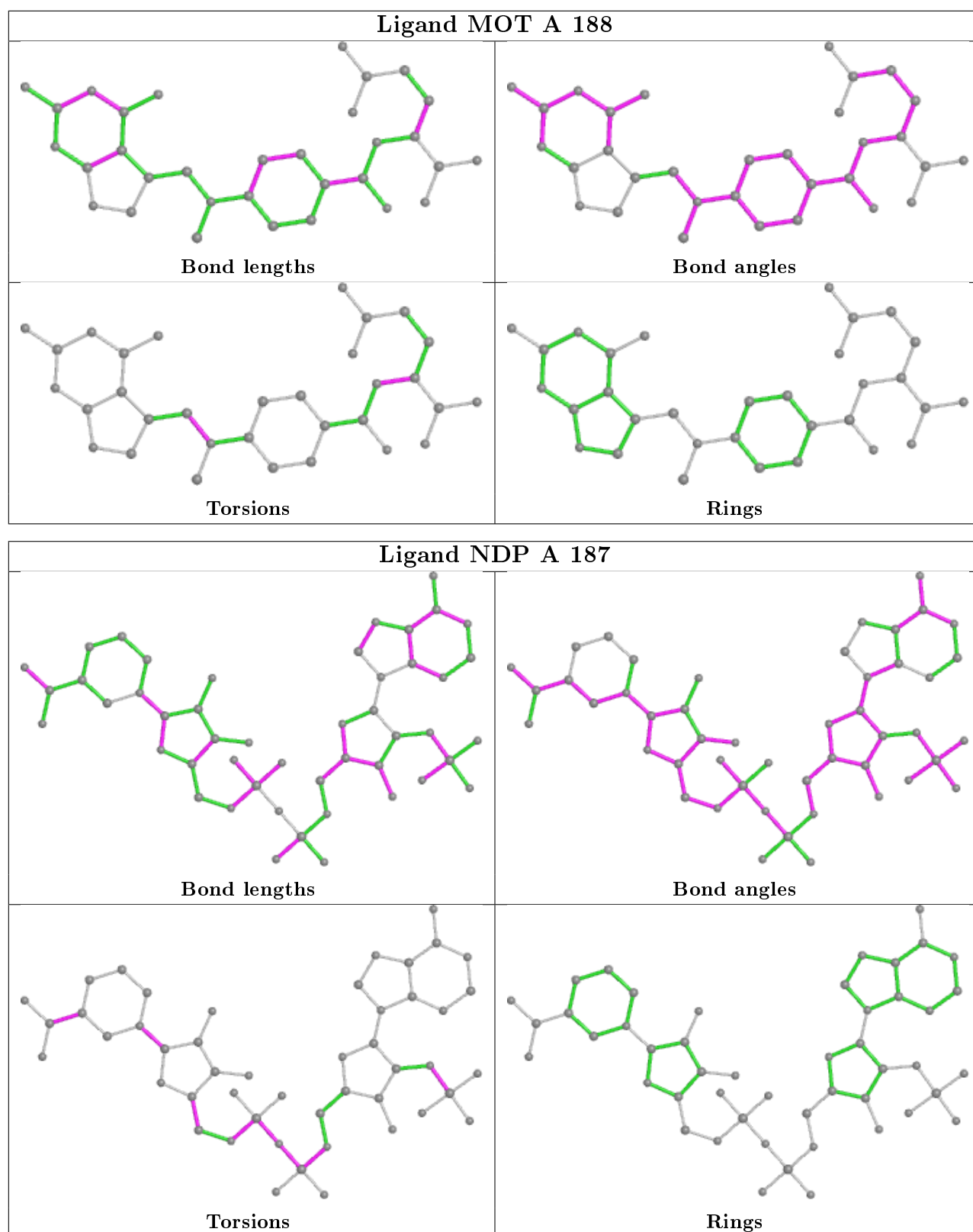
Mol	Chain	Res	Type	Atoms
2	A	187	NDP	C5D-O5D-PN-O1N
2	A	187	NDP	O4D-C1D-N1N-C2N
2	A	187	NDP	PN-O3-PA-O2A
2	A	187	NDP	C2D-C1D-N1N-C2N
3	A	188	MOT	C6-C9-N10-C14
2	A	187	NDP	C2N-C3N-C7N-N7N

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	188	MOT	1	0
2	A	187	NDP	3	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.