



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:37 PM UTC

PDB ID : 1HFR / pdb_00001hfr
Title : COMPARISON OF TERNARY CRYSTAL COMPLEXES OF HUMAN DI-HYDROFOLATE REDUCTASE WITH NADPH AND A CLASSICAL AN-TITUMOR FUOPYRIMDINE
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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

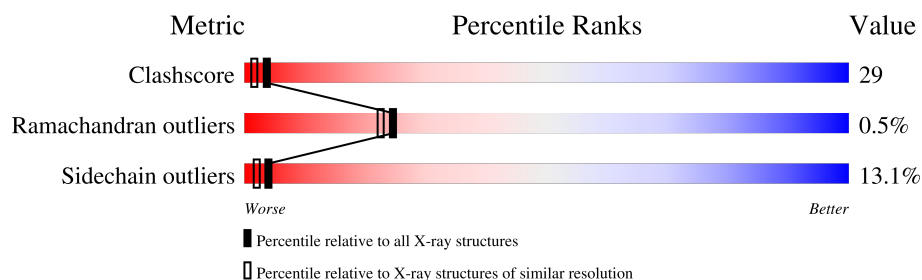
1 Overall quality at a glance

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	17% 49% 29% 5%

2 Entry composition [i](#)

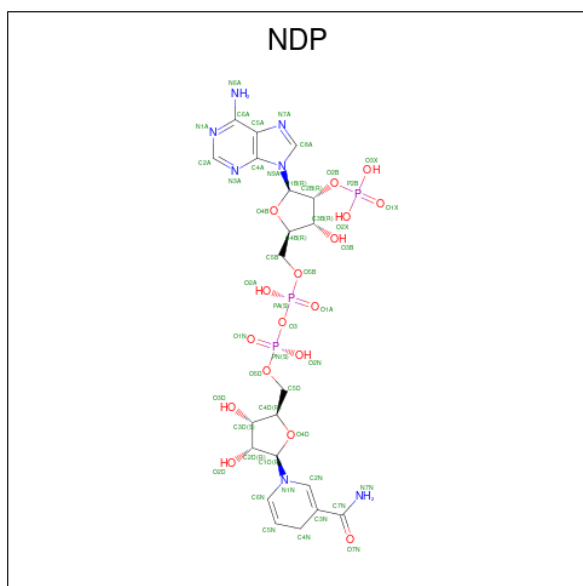
There are 4 unique types of molecules in this entry. The entry contains 1617 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

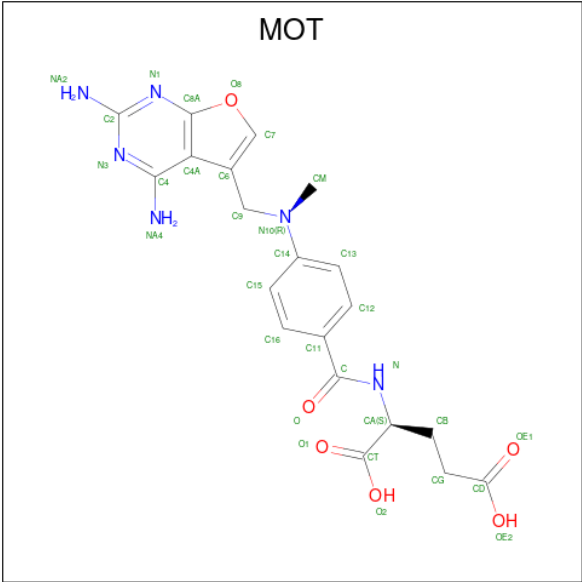
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1502	963	253	279	7			

- 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
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- 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.

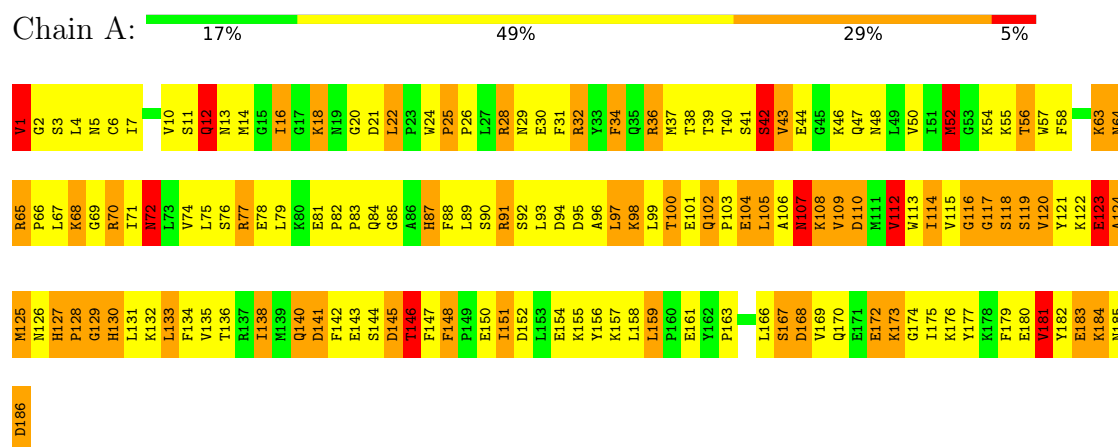
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		

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	H 3	Depositor
Cell constants a, b, c, α , β , γ	86.90Å 86.90Å 77.09Å 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 ²)	24.0	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	1.75	14/1537 (0.9%)	3.29	257/2073 (12.4%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	LEU	N-CA	8.25	1.56	1.46
1	A	18	LYS	C-O	-7.03	1.16	1.23
1	A	55	LYS	CA-C	-6.02	1.44	1.52
1	A	56	THR	CA-CB	5.92	1.62	1.53
1	A	5	ASN	C-O	-5.81	1.16	1.23
1	A	21	ASP	N-CA	5.67	1.54	1.46
1	A	175	ILE	N-CA	5.56	1.52	1.46
1	A	40	THR	N-CA	5.54	1.53	1.46
1	A	168	ASP	N-CA	5.52	1.52	1.45
1	A	70	ARG	N-CA	-5.41	1.38	1.45
1	A	130	HIS	CG-ND1	5.41	1.44	1.38
1	A	16	ILE	C-N	5.33	1.40	1.33
1	A	38	THR	CB-OG1	5.24	1.52	1.43
1	A	16	ILE	CA-CB	5.17	1.61	1.54

All (257) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ASP	CA-CB-CG	-20.44	92.16	112.60
1	A	126	ASN	CA-CB-CG	15.70	128.30	112.60
1	A	25	PRO	CB-CA-C	13.90	127.88	110.92
1	A	168	ASP	CA-CB-CG	-13.69	98.91	112.60
1	A	116	GLY	CA-C-N	12.83	144.80	121.70
1	A	116	GLY	C-N-CA	12.83	144.80	121.70
1	A	72	ASN	CA-C-O	-12.21	107.30	120.36
1	A	77	ARG	CD-NE-CZ	-12.00	107.60	124.40
1	A	154	GLU	CB-CG-CD	11.31	131.83	112.60
1	A	101	GLU	CB-CG-CD	10.52	130.48	112.60
1	A	56	THR	CA-CB-OG1	-10.38	94.03	109.60
1	A	1	VAL	CA-CB-CG1	10.19	127.72	110.40
1	A	115	VAL	CA-C-O	-9.91	110.09	119.91
1	A	72	ASN	O-C-N	9.84	134.43	123.22
1	A	108	LYS	N-CA-C	9.62	125.15	113.41
1	A	143	GLU	CA-C-O	-9.45	110.59	120.80
1	A	152	ASP	CA-C-O	-9.31	110.62	120.58
1	A	158	LEU	CA-C-O	-9.28	110.11	120.69
1	A	13	ASN	OD1-CG-ND2	-9.12	113.48	122.60
1	A	72	ASN	OD1-CG-ND2	-8.99	113.61	122.60
1	A	66	PRO	N-CD-CG	-8.91	93.11	103.80
1	A	64	ASN	CA-C-O	-8.87	109.49	119.95
1	A	77	ARG	NH1-CZ-NH2	8.84	130.79	119.30
1	A	91	ARG	CD-NE-CZ	-8.79	112.09	124.40
1	A	146	THR	CA-CB-CG2	8.78	125.43	110.50
1	A	136	THR	CA-C-O	-8.76	110.99	120.36
1	A	42	SER	CA-C-O	-8.73	107.68	119.12
1	A	1	VAL	CB-CA-C	8.73	127.98	111.40
1	A	77	ARG	CA-CB-CG	-8.68	96.73	114.10
1	A	11	SER	O-C-N	-8.68	111.98	122.65
1	A	132	LYS	CA-C-O	-8.65	111.36	120.70
1	A	91	ARG	CA-CB-CG	-8.61	96.89	114.10
1	A	70	ARG	CA-C-O	-8.59	111.39	121.44
1	A	107	ASN	CA-CB-CG	-8.59	104.01	112.60
1	A	120	VAL	N-CA-C	-8.56	102.52	110.82
1	A	176	LYS	CA-C-O	-8.53	111.34	120.80
1	A	77	ARG	NE-CZ-NH1	-8.46	113.04	121.50
1	A	30	GLU	CB-CG-CD	8.45	126.97	112.60
1	A	65	ARG	CD-NE-CZ	8.44	136.22	124.40
1	A	125	MET	CA-C-O	-8.38	110.63	120.10
1	A	57	TRP	O-C-N	-8.29	113.47	122.09
1	A	181	VAL	CA-CB-CG2	8.26	124.45	110.40
1	A	146	THR	CB-CA-C	8.24	124.07	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	TYR	O-C-N	8.21	132.61	123.25
1	A	125	MET	N-CA-C	8.19	121.12	111.71
1	A	72	ASN	CB-CG-ND2	8.13	128.59	116.40
1	A	64	ASN	OD1-CG-ND2	8.11	130.71	122.60
1	A	134	PHE	CA-C-O	-8.11	112.11	120.54
1	A	11	SER	CA-C-O	7.97	131.11	121.94
1	A	58	PHE	CA-CB-CG	-7.97	105.83	113.80
1	A	110	ASP	O-C-N	-7.92	112.05	122.59
1	A	95	ASP	CA-CB-CG	-7.81	104.79	112.60
1	A	78	GLU	CA-CB-CG	7.73	129.56	114.10
1	A	83	PRO	CB-CA-C	7.73	121.07	110.95
1	A	177	TYR	CA-C-O	-7.64	113.08	121.33
1	A	87	HIS	ND1-CE1-NE2	-7.61	100.79	108.40
1	A	70	ARG	NE-CZ-NH2	-7.61	112.35	119.20
1	A	44	GLU	CB-CG-CD	7.61	125.53	112.60
1	A	48	ASN	OD1-CG-ND2	-7.58	115.03	122.60
1	A	18	LYS	CA-C-O	-7.55	111.00	120.28
1	A	138	ILE	N-CA-C	-7.44	96.12	107.73
1	A	138	ILE	CA-C-O	-7.43	111.69	120.75
1	A	84	GLN	CA-C-O	-7.37	112.93	120.96
1	A	12	GLN	OE1-CD-NE2	7.33	129.93	122.60
1	A	110	ASP	CB-CA-C	7.32	124.98	110.42
1	A	176	LYS	O-C-N	7.29	131.72	123.19
1	A	30	GLU	CA-C-N	7.28	133.03	120.58
1	A	30	GLU	C-N-CA	7.28	133.03	120.58
1	A	169	VAL	CA-CB-CG2	7.28	122.77	110.40
1	A	3	SER	CA-C-O	-7.26	113.03	121.16
1	A	145	ASP	CB-CA-C	7.23	121.13	109.27
1	A	181	VAL	N-CA-CB	7.22	122.06	111.52
1	A	74	VAL	O-C-N	-7.21	115.79	123.14
1	A	181	VAL	CA-C-O	7.20	127.99	120.36
1	A	39	THR	CA-CB-OG1	-7.18	98.83	109.60
1	A	118	SER	N-CA-C	7.14	120.89	111.75
1	A	143	GLU	CB-CG-CD	7.14	124.74	112.60
1	A	22	LEU	CA-C-O	-7.13	113.30	120.64
1	A	29	ASN	N-CA-C	-7.10	104.65	113.38
1	A	183	GLU	CA-C-N	7.08	133.71	122.59
1	A	183	GLU	C-N-CA	7.08	133.71	122.59
1	A	79	LEU	CA-C-O	-7.07	113.86	121.56
1	A	31	PHE	N-CA-CB	7.06	120.72	110.20
1	A	143	GLU	CB-CA-C	-7.05	100.26	110.06
1	A	40	THR	CA-CB-OG1	-7.02	99.07	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	LYS	N-CA-CB	-7.02	100.22	110.47
1	A	70	ARG	NH1-CZ-NH2	7.01	128.41	119.30
1	A	163	PRO	CB-CA-C	-6.99	102.84	111.64
1	A	32	ARG	CA-CB-CG	-6.96	100.17	114.10
1	A	109	VAL	N-CA-CB	-6.96	102.64	110.99
1	A	110	ASP	CB-CG-OD2	6.91	134.30	118.40
1	A	41	SER	CA-CB-OG	-6.90	97.31	111.10
1	A	3	SER	O-C-N	6.88	131.29	122.89
1	A	52	MET	CA-C-O	-6.83	113.86	121.51
1	A	71	ILE	N-CA-CB	6.79	118.74	111.00
1	A	5	ASN	CA-CB-CG	6.78	119.38	112.60
1	A	92	SER	O-C-N	-6.78	116.16	123.42
1	A	97	LEU	N-CA-C	-6.76	103.37	111.69
1	A	148	PHE	CA-C-O	-6.74	113.35	120.23
1	A	30	GLU	N-CA-C	-6.74	103.74	112.23
1	A	42	SER	CA-C-N	6.74	132.52	122.75
1	A	42	SER	C-N-CA	6.74	132.52	122.75
1	A	173	LYS	CB-CA-C	-6.72	101.10	111.66
1	A	25	PRO	N-CA-C	-6.68	102.55	110.70
1	A	57	TRP	CA-C-O	6.64	128.01	120.90
1	A	101	GLU	CB-CA-C	-6.58	98.65	110.37
1	A	28	ARG	NE-CZ-NH2	6.57	125.11	119.20
1	A	180	GLU	CB-CG-CD	6.57	123.76	112.60
1	A	40	THR	N-CA-C	6.55	119.21	109.59
1	A	91	ARG	O-C-N	6.54	131.40	122.37
1	A	154	GLU	CG-CD-OE1	6.49	133.32	118.40
1	A	176	LYS	CA-CB-CG	-6.44	101.22	114.10
1	A	102	GLN	N-CA-C	-6.44	100.29	109.62
1	A	50	VAL	N-CA-CB	6.42	119.99	111.64
1	A	98	LYS	CA-C-N	6.41	131.43	120.72
1	A	98	LYS	C-N-CA	6.41	131.43	120.72
1	A	30	GLU	O-C-N	-6.38	113.78	122.33
1	A	69	GLY	O-C-N	6.33	129.85	122.45
1	A	110	ASP	OD1-CG-OD2	-6.33	107.72	122.90
1	A	140	GLN	OE1-CD-NE2	6.32	128.92	122.60
1	A	39	THR	CA-C-O	-6.26	113.29	120.24
1	A	180	GLU	CA-C-N	6.26	131.69	122.99
1	A	180	GLU	C-N-CA	6.26	131.69	122.99
1	A	7	ILE	CA-C-N	6.26	131.24	122.23
1	A	7	ILE	C-N-CA	6.26	131.24	122.23
1	A	157	LYS	CA-CB-CG	-6.25	101.60	114.10
1	A	83	PRO	O-C-N	-6.25	115.38	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ALA	CA-C-N	6.24	131.24	120.58
1	A	96	ALA	C-N-CA	6.24	131.24	120.58
1	A	180	GLU	CG-CD-OE2	6.23	132.72	118.40
1	A	129	GLY	O-C-N	6.21	132.14	122.70
1	A	85	GLY	O-C-N	-6.16	116.25	122.65
1	A	91	ARG	NH1-CZ-NH2	6.14	127.28	119.30
1	A	7	ILE	CB-CA-C	6.12	119.95	110.28
1	A	32	ARG	CA-C-N	6.11	128.75	120.44
1	A	32	ARG	C-N-CA	6.11	128.75	120.44
1	A	5	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	A	126	ASN	CB-CG-OD1	6.08	132.96	120.80
1	A	167	SER	CA-C-N	-6.07	111.69	122.74
1	A	167	SER	C-N-CA	-6.07	111.69	122.74
1	A	169	VAL	CA-C-O	6.07	128.45	120.98
1	A	83	PRO	CA-C-N	6.07	129.73	121.05
1	A	83	PRO	C-N-CA	6.07	129.73	121.05
1	A	144	SER	CA-CB-OG	-6.07	98.97	111.10
1	A	110	ASP	CA-C-O	6.06	129.18	120.51
1	A	54	LYS	CA-C-O	-6.06	114.42	120.90
1	A	122	LYS	CA-CB-CG	-6.06	101.98	114.10
1	A	64	ASN	CB-CA-C	-6.05	101.27	111.02
1	A	18	LYS	CA-CB-CG	-6.04	102.02	114.10
1	A	161	GLU	CB-CG-CD	6.03	122.86	112.60
1	A	152	ASP	N-CA-CB	-6.03	100.62	110.21
1	A	2	GLY	CA-C-N	6.02	129.41	120.87
1	A	2	GLY	C-N-CA	6.02	129.41	120.87
1	A	179	PHE	CA-C-O	-5.98	113.91	120.43
1	A	69	GLY	CA-C-O	-5.97	112.19	119.06
1	A	125	MET	CA-CB-CG	-5.95	102.19	114.10
1	A	181	VAL	CB-CA-C	5.95	119.02	110.33
1	A	179	PHE	CA-CB-CG	5.92	119.72	113.80
1	A	141	ASP	CB-CG-OD1	-5.90	104.83	118.40
1	A	71	ILE	CA-C-O	-5.89	113.75	120.65
1	A	112	VAL	CG1-CB-CG2	5.89	123.76	110.80
1	A	185	ASN	N-CA-CB	5.88	120.44	110.49
1	A	20	GLY	CA-C-N	-5.88	112.75	122.39
1	A	20	GLY	C-N-CA	-5.88	112.75	122.39
1	A	77	ARG	CG-CD-NE	-5.87	99.09	112.00
1	A	135	VAL	CA-C-O	-5.83	114.29	120.53
1	A	124	ALA	N-CA-C	-5.81	104.94	111.28
1	A	68	LYS	CA-CB-CG	-5.79	102.52	114.10
1	A	90	SER	O-C-N	5.79	130.17	123.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	SER	N-CA-C	5.78	118.84	110.28
1	A	12	GLN	CG-CD-OE1	-5.78	109.24	120.80
1	A	71	ILE	O-C-N	5.77	129.98	122.94
1	A	155	LYS	CA-C-O	-5.76	112.73	119.24
1	A	138	ILE	CA-CB-CG1	5.76	120.19	110.40
1	A	34	PHE	CA-CB-CG	-5.76	108.04	113.80
1	A	65	ARG	CB-CG-CD	5.76	124.54	111.30
1	A	29	ASN	N-CA-CB	5.74	119.09	110.53
1	A	186	ASP	CA-C-O	-5.74	103.77	121.00
1	A	112	VAL	N-CA-CB	5.72	119.07	111.64
1	A	154	GLU	CA-CB-CG	-5.72	102.67	114.10
1	A	113	TRP	N-CA-C	5.70	118.02	108.73
1	A	112	VAL	CA-CB-CG1	5.70	120.08	110.40
1	A	36	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	A	122	LYS	CA-C-N	5.69	130.21	120.71
1	A	122	LYS	C-N-CA	5.69	130.21	120.71
1	A	147	PHE	CA-C-O	-5.64	114.86	121.46
1	A	115	VAL	O-C-N	5.63	127.96	122.05
1	A	30	GLU	CB-CA-C	5.60	121.80	110.38
1	A	64	ASN	O-C-N	5.60	129.15	122.26
1	A	172	GLU	CA-CB-CG	5.59	125.29	114.10
1	A	181	VAL	O-C-N	-5.59	117.16	123.20
1	A	112	VAL	O-C-N	5.57	129.10	123.20
1	A	141	ASP	O-C-N	5.56	129.60	123.16
1	A	126	ASN	N-CA-C	-5.55	106.55	113.38
1	A	6	CYS	N-CA-CB	5.54	120.56	111.08
1	A	181	VAL	CA-CB-CG1	5.54	119.82	110.40
1	A	98	LYS	O-C-N	-5.53	115.75	122.22
1	A	44	GLU	CA-C-O	5.50	127.24	121.19
1	A	112	VAL	CA-CB-CG2	-5.47	101.09	110.40
1	A	90	SER	CA-C-O	-5.46	115.23	121.40
1	A	151	ILE	CA-C-O	-5.46	114.54	120.71
1	A	67	LEU	CB-CA-C	5.45	118.01	110.16
1	A	134	PHE	N-CA-C	-5.45	98.88	108.20
1	A	105	LEU	N-CA-C	5.45	119.99	113.23
1	A	91	ARG	NE-CZ-NH1	-5.44	116.06	121.50
1	A	132	LYS	O-C-N	5.44	130.30	123.23
1	A	128	PRO	CA-C-N	-5.44	110.30	123.46
1	A	128	PRO	C-N-CA	-5.44	110.30	123.46
1	A	70	ARG	CD-NE-CZ	-5.42	116.81	124.40
1	A	173	LYS	CA-CB-CG	-5.38	103.33	114.10
1	A	74	VAL	CA-C-O	5.37	126.84	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	HIS	ND1-CE1-NE2	-5.35	103.05	108.40
1	A	42	SER	CB-CA-C	-5.34	99.96	110.11
1	A	177	TYR	N-CA-C	-5.34	100.95	109.07
1	A	71	ILE	N-CA-C	-5.33	100.08	108.23
1	A	43	VAL	CA-C-O	-5.32	114.63	120.43
1	A	70	ARG	CA-C-N	5.31	129.00	122.37
1	A	70	ARG	C-N-CA	5.31	129.00	122.37
1	A	150	GLU	CB-CG-CD	5.30	121.61	112.60
1	A	127	HIS	N-CA-C	-5.29	102.48	109.84
1	A	117	GLY	CA-C-N	-5.29	112.66	120.38
1	A	117	GLY	C-N-CA	-5.29	112.66	120.38
1	A	109	VAL	N-CA-C	5.28	115.92	108.36
1	A	138	ILE	O-C-N	5.28	129.31	122.77
1	A	123	GLU	N-CA-CB	-5.27	102.33	110.13
1	A	151	ILE	O-C-N	5.24	128.93	122.95
1	A	155	LYS	N-CA-CB	5.24	117.56	110.59
1	A	90	SER	N-CA-CB	5.24	120.80	111.69
1	A	182	TYR	CA-C-O	-5.24	115.19	121.11
1	A	88	PHE	O-C-N	5.23	129.34	123.27
1	A	77	ARG	O-C-N	5.22	128.78	122.35
1	A	147	PHE	N-CA-CB	-5.21	102.76	111.20
1	A	98	LYS	N-CA-CB	5.19	118.21	110.22
1	A	84	GLN	O-C-N	5.18	129.27	123.06
1	A	150	GLU	CG-CD-OE1	-5.17	106.50	118.40
1	A	56	THR	N-CA-CB	5.17	117.56	110.07
1	A	119	SER	O-C-N	5.17	128.62	122.27
1	A	12	GLN	O-C-N	-5.14	116.20	122.22
1	A	39	THR	CB-CA-C	-5.14	101.29	110.70
1	A	5	ASN	N-CA-CB	-5.12	102.78	111.69
1	A	145	ASP	N-CA-C	-5.11	106.97	114.39
1	A	125	MET	O-C-N	5.11	128.19	122.22
1	A	58	PHE	CD1-CG-CD2	5.09	126.24	118.60
1	A	131	LEU	CB-CA-C	5.08	119.69	109.38
1	A	100	THR	CA-C-N	5.07	131.28	122.56
1	A	100	THR	C-N-CA	5.07	131.28	122.56
1	A	113	TRP	CA-C-N	5.07	128.71	122.37
1	A	113	TRP	C-N-CA	5.07	128.71	122.37
1	A	7	ILE	CA-C-O	-5.07	114.91	120.43
1	A	95	ASP	CA-C-N	-5.06	113.10	120.29
1	A	95	ASP	C-N-CA	-5.06	113.10	120.29
1	A	159	LEU	O-C-N	5.05	128.06	121.64
1	A	136	THR	N-CA-C	-5.04	100.51	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	GLY	O-C-N	5.03	129.24	122.70
1	A	123	GLU	OE1-CD-OE2	5.03	134.98	122.90
1	A	110	ASP	CA-C-N	5.02	131.17	122.64
1	A	110	ASP	C-N-CA	5.02	131.17	122.64

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	1511	91	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	1557	91	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 29.

All (91) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:168:ASP:OD1	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:HD12	1:A:166:LEU:N	2.09	0.68
1:A:114:ILE:HD13	1:A:124:ALA:HB2	1.75	0.68
1:A:166:LEU:N	1:A:166:LEU:CD1	2.58	0.66
1:A:116:GLY:HA3	2:A:187:NDP:H5N	1.78	0.63
1:A:186:ASP:OD1	1:A:186:ASP:C	2.41	0.63
1:A:99:LEU:HD22	1:A:105:LEU:CD1	2.28	0.62
1:A:36:ARG:NH1	1:A:37:MET:HE3	2.13	0.62
1:A:141:ASP:OD1	1:A:141:ASP:N	2.17	0.61
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:130:HIS:HE1	1:A:183:GLU:CG	2.15	0.59
1:A:168:ASP:O	1:A:170:GLN:NE2	2.30	0.59
1:A:156:TYR:CZ	1:A:184:LYS:HD3	2.37	0.59
1:A:99:LEU:O	1:A:99:LEU:HD23	2.03	0.59
1:A:123:GLU:OE1	2:A:187:NDP:N6A	2.37	0.58
1:A:1:VAL:HG21	1:A:106:ALA:O	2.04	0.58
1:A:47:GLN:O	1:A:109:VAL:HA	2.04	0.58
1:A:114:ILE:HD13	1:A:124:ALA:CB	2.34	0.58
1:A:103:PRO:O	1:A:104:GLU:C	2.46	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:ND2	1:A:107:ASN:N	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:PRO:O	1:A:173:LYS:HE3	2.08	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:140:GLN:C	1:A:141:ASP:OD1	2.53	0.51
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:125:MET:HE3	1:A:133:LEU:HD21	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:107:ASN:HD22	1:A:107:ASN:C	2.20	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:172:GLU:C	1:A:174:GLY:N	2.71	0.47
1:A:36:ARG:CZ	1:A:37:MET:HE3	2.45	0.47
1:A:34:PHE:CD1	1:A:34:PHE:C	2.93	0.46
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
1:A:166:LEU:H	1:A:166:LEU:HD13	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: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:102:GLN:O	1:A:103:PRO:C	2.60	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:75:LEU:HD23	1:A:75:LEU:HA	1.76	0.41
1:A:151:ILE:HD13	1:A:151:ILE:HG21	1.88	0.41
1:A:24:TRP:HB3	1:A:142:PHE:CZ	2.55	0.41
1:A:76:SER:HB3	1:A:89:LEU:HD11	2.01	0.41
1:A:97:LEU:O	1:A:98:LYS:C	2.62	0.41
1:A:156:TYR:CD1	1:A:184:LYS:HB2	2.56	0.41
1:A:102:GLN:C	1:A:104:GLU:N	2.77	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:172:GLU:O	1:A:173:LYS:C	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ALA:O	1:A:127:HIS:HB3	2.21	0.40
1:A:127:HIS:CG	1:A:128:PRO:HD2	2.57	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%)	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	168/168 (100%)	146 (87%)	22 (13%)	4 2

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL

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Mol	Chain	Res	Type
1	A	12	GLN
1	A	18	LYS
1	A	22	LEU
1	A	42	SER
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	114	ILE
1	A	118	SER
1	A	119	SER
1	A	123	GLU
1	A	133	LEU
1	A	138	ILE
1	A	146	THR
1	A	167	SER
1	A	181	VAL
1	A	184	LYS

Sometimes 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
1	A	87	HIS
1	A	107	ASN
1	A	127	HIS
1	A	185	ASN

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	$\# Z > 2$
3	MOT	A	188	-	34,34,34	3.57	13 (38%)	41,48,48	3.81	25 (60%)
2	NDP	A	187	-	51,52,52	2.94	22 (43%)	71,80,80	2.56	32 (45%)

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	-	-	2/25/25/25	0/3/3/3
2	NDP	A	187	-	-	12/34/77/77	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	188	MOT	O8-C8A	-11.71	1.21	1.37
2	A	187	NDP	P2B-O2B	9.34	1.75	1.59
3	A	188	MOT	C4A-C4	-8.80	1.32	1.42
2	A	187	NDP	O4B-C4B	-8.71	1.25	1.45
3	A	188	MOT	O8-C7	-6.25	1.20	1.38
2	A	187	NDP	C5A-C6A	5.85	1.57	1.41
3	A	188	MOT	C11-C	-5.73	1.37	1.50
3	A	188	MOT	C4-N3	-5.49	1.27	1.35
2	A	187	NDP	O4D-C1D	5.20	1.54	1.42
2	A	187	NDP	C5A-C4A	-5.00	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	188	MOT	C2-N3	-4.60	1.27	1.35
2	A	187	NDP	C3B-C4B	4.38	1.64	1.53
3	A	188	MOT	C4A-C8A	-4.32	1.34	1.39
2	A	187	NDP	O3B-C3B	4.06	1.53	1.43
2	A	187	NDP	C6A-N1A	-4.00	1.24	1.35
3	A	188	MOT	C15-C14	-3.65	1.32	1.39
3	A	188	MOT	C8A-N1	3.61	1.37	1.32
2	A	187	NDP	C1D-N1N	3.59	1.56	1.46
2	A	187	NDP	PN-O1N	-3.38	1.39	1.50
2	A	187	NDP	PA-O3	-3.27	1.56	1.59
2	A	187	NDP	C3D-C4D	3.11	1.60	1.53
2	A	187	NDP	P2B-O3X	-2.94	1.43	1.54
3	A	188	MOT	OE2-CD	-2.91	1.21	1.30
2	A	187	NDP	PA-O1A	-2.91	1.40	1.50
3	A	188	MOT	C16-C15	-2.83	1.34	1.38
2	A	187	NDP	C4A-N9A	-2.79	1.31	1.37
2	A	187	NDP	PN-O2N	-2.65	1.43	1.55
2	A	187	NDP	C2B-C1B	2.57	1.59	1.53
2	A	187	NDP	PN-O3	-2.46	1.56	1.59
2	A	187	NDP	PN-O5D	2.26	1.68	1.59
3	A	188	MOT	CB-CA	2.22	1.58	1.53
2	A	187	NDP	O7N-C7N	-2.21	1.19	1.24
2	A	187	NDP	C5B-C4B	2.19	1.58	1.51
2	A	187	NDP	C4A-N3A	2.18	1.38	1.34
3	A	188	MOT	CM-N10	2.05	1.49	1.46

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188	MOT	C8A-O8-C7	10.50	112.50	105.80
3	A	188	MOT	C2-N3-C4	7.86	126.71	117.28
3	A	188	MOT	O8-C8A-C4A	6.45	114.17	110.00
3	A	188	MOT	O8-C8A-N1	6.42	122.62	119.20
3	A	188	MOT	C4A-C4-NA4	6.40	131.86	123.40
3	A	188	MOT	O8-C7-C6	-6.16	108.86	112.91
2	A	187	NDP	O4D-C1D-N1N	-5.81	97.01	108.08
2	A	187	NDP	C4B-O4B-C1B	5.56	121.74	109.47
2	A	187	NDP	O3-PN-O1N	5.25	126.49	110.70
2	A	187	NDP	C3N-C2N-N1N	-5.18	115.59	123.20
2	A	187	NDP	O3D-C3D-C4D	-5.12	96.38	111.08
3	A	188	MOT	O2-CT-CA	5.08	130.71	113.51
3	A	188	MOT	O-C-N	-5.03	112.90	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	187	NDP	O4B-C1B-C2B	-4.94	98.08	106.59
2	A	187	NDP	C6N-N1N-C2N	4.92	124.59	119.32
3	A	188	MOT	CB-CA-N	-4.68	101.64	110.91
2	A	187	NDP	C5B-C4B-C3B	-4.62	98.59	115.21
3	A	188	MOT	C16-C15-C14	4.57	126.08	120.30
2	A	187	NDP	O3B-C3B-C4B	-4.39	98.46	111.08
2	A	187	NDP	C5A-C4A-N9A	4.34	110.54	105.81
3	A	188	MOT	NA2-C2-N3	4.02	123.25	117.22
3	A	188	MOT	CM-N10-C9	-4.00	104.52	114.49
3	A	188	MOT	NA4-C4-N3	-3.90	111.76	117.03
3	A	188	MOT	CM-N10-C14	3.89	126.04	119.59
2	A	187	NDP	PN-O5D-C5D	3.84	143.38	121.35
2	A	187	NDP	O4B-C1B-N9A	3.75	115.29	108.09
3	A	188	MOT	C16-C11-C12	-3.73	113.82	118.57
2	A	187	NDP	O2X-P2B-O2B	-3.49	92.25	105.85
2	A	187	NDP	O3-PA-O1A	-3.48	100.23	110.70
2	A	187	NDP	P2B-O2B-C2B	-3.47	114.17	123.43
3	A	188	MOT	O1-CT-CA	-3.25	111.78	122.26
3	A	188	MOT	C4A-C4-N3	-3.06	116.35	121.62
2	A	187	NDP	O4D-C4D-C5D	3.03	119.05	109.33
3	A	188	MOT	O-C-C11	2.92	126.69	120.90
3	A	188	MOT	O2-CT-O1	-2.91	117.48	124.08
3	A	188	MOT	CB-CG-CD	-2.87	104.83	112.49
2	A	187	NDP	O3X-P2B-O1X	2.87	122.00	110.83
2	A	187	NDP	C5A-C6A-N6A	-2.83	116.29	123.29
3	A	188	MOT	C13-C12-C11	2.81	123.80	120.80
2	A	187	NDP	O2N-PN-O5D	-2.80	94.86	107.57
2	A	187	NDP	C4A-N9A-C1B	2.78	133.13	126.63
2	A	187	NDP	O5B-C5B-C4B	-2.70	99.80	108.99
3	A	188	MOT	N3-C2-N1	-2.60	121.50	125.48
2	A	187	NDP	O5D-C5D-C4D	-2.56	100.27	108.99
3	A	188	MOT	CA-N-C	2.49	127.53	121.56
2	A	187	NDP	N6A-C6A-N1A	2.46	123.85	118.38
2	A	187	NDP	O4B-C4B-C3B	-2.45	100.29	105.15
2	A	187	NDP	O7N-C7N-C3N	-2.34	116.50	120.90
3	A	188	MOT	C15-C14-C13	-2.33	114.73	119.18
2	A	187	NDP	C2B-C3B-C4B	-2.28	97.09	101.99
2	A	187	NDP	C1B-N9A-C8A	-2.22	122.17	127.09
2	A	187	NDP	C2D-C1D-N1N	2.08	118.42	113.31
2	A	187	NDP	C6A-C5A-N7A	2.06	136.05	132.09
2	A	187	NDP	C1D-N1N-C2N	-2.03	117.79	121.14
2	A	187	NDP	C5A-C4A-N3A	-2.01	123.94	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188	MOT	C2-N1-C8A	-2.01	113.16	115.96
2	A	187	NDP	O2B-P2B-O1X	-2.01	102.19	109.33

There are no chirality outliers.

All (14) torsion outliers are listed below:

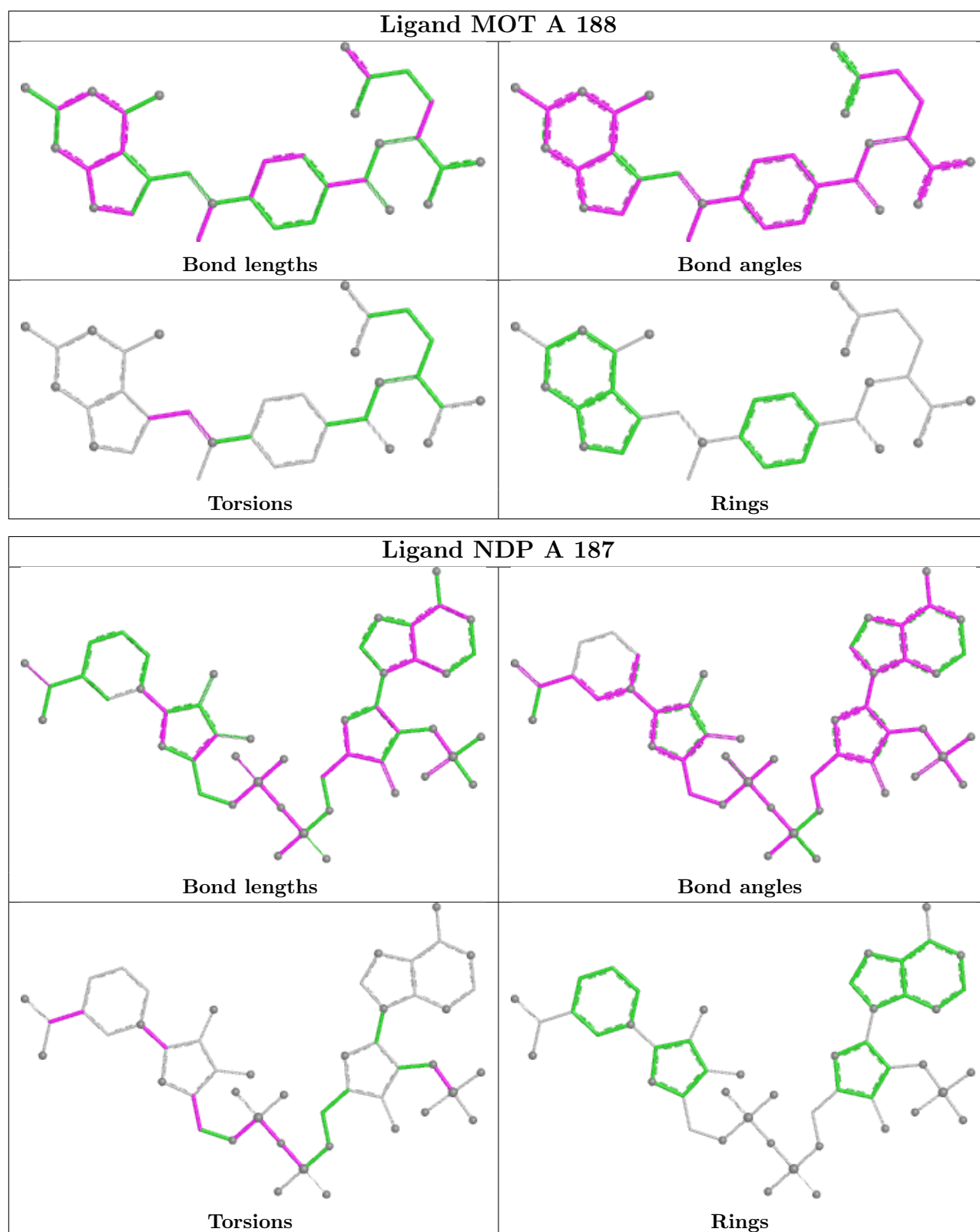
Mol	Chain	Res	Type	Atoms
2	A	187	NDP	C5D-O5D-PN-O2N
2	A	187	NDP	C3D-C4D-C5D-O5D
2	A	187	NDP	PA-O3-PN-O1N
2	A	187	NDP	C5D-O5D-PN-O3
2	A	187	NDP	C5D-O5D-PN-O1N
3	A	188	MOT	C7-C6-C9-N10
2	A	187	NDP	PN-O3-PA-O2A
2	A	187	NDP	O4D-C1D-N1N-C2N
2	A	187	NDP	C2N-C3N-C7N-N7N
2	A	187	NDP	C2D-C1D-N1N-C2N
2	A	187	NDP	C2B-O2B-P2B-O3X
3	A	188	MOT	C6-C9-N10-C14
2	A	187	NDP	PN-O3-PA-O1A
2	A	187	NDP	PA-O3-PN-O2N

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.