



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:02 PM UTC

PDB ID : 1HFQ / pdb_00001hfq
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

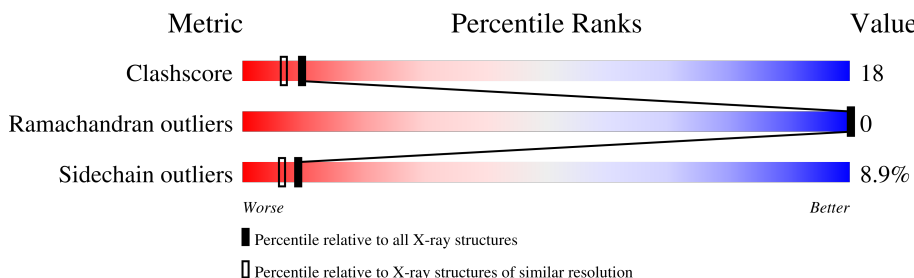
1 Overall quality at a glance

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	15% 59% 24% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1628 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.

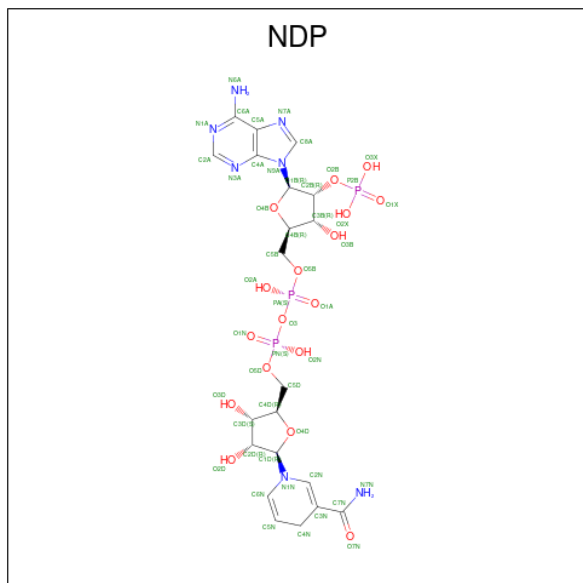
- Molecule 1 is a protein called DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1497	957	253	280	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

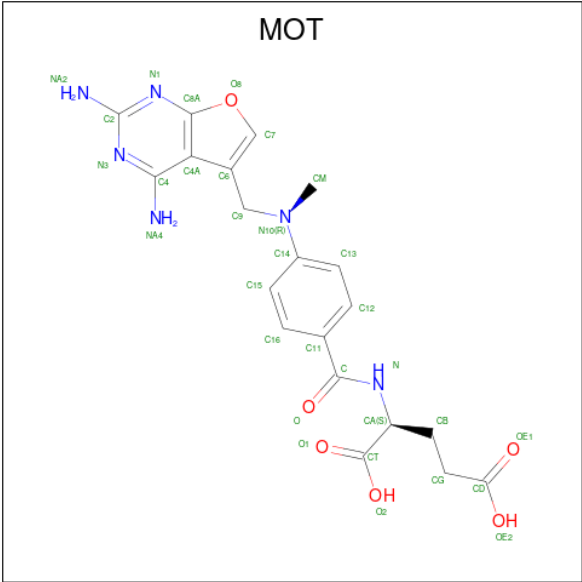
Chain	Residue	Modelled	Actual	Comment	Reference
A	31	SER	PHE	engineered mutation	UNP P00374

- 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: $C_{20}H_{22}N_6O_6$).

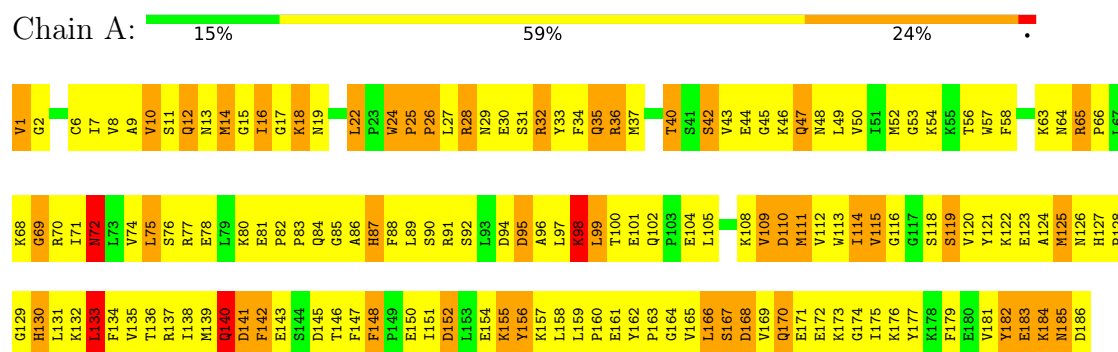


3 Residue-property plots

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	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}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.175 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1628	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: 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	2.55	88/1531 (5.7%)	3.77	331/2065 (16.0%)

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 (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	ALA	C-O	12.75	1.39	1.24
1	A	34	PHE	N-CA	11.41	1.60	1.46
1	A	119	SER	CB-OG	9.86	1.61	1.42
1	A	16	ILE	CA-CB	9.71	1.66	1.54
1	A	172	GLU	N-CA	9.50	1.57	1.46
1	A	176	LYS	N-CA	9.27	1.56	1.45
1	A	17	GLY	CA-C	9.19	1.60	1.51
1	A	136	THR	C-O	9.03	1.35	1.24
1	A	16	ILE	CB-CG1	8.95	1.71	1.53
1	A	114	ILE	C-O	8.92	1.33	1.24
1	A	48	ASN	CA-C	8.48	1.64	1.52
1	A	57	TRP	C-O	8.24	1.33	1.24
1	A	49	LEU	N-CA	8.15	1.56	1.46
1	A	71	ILE	C-O	7.94	1.32	1.24
1	A	147	PHE	C-O	7.88	1.33	1.23
1	A	29	ASN	C-N	-7.70	1.24	1.33
1	A	97	LEU	N-CA	7.60	1.56	1.46
1	A	146	THR	CA-C	7.60	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	VAL	CA-C	7.56	1.62	1.52
1	A	168	ASP	N-CA	7.46	1.54	1.45
1	A	10	VAL	N-CA	-7.44	1.37	1.46
1	A	52	MET	CA-C	7.28	1.61	1.52
1	A	135	VAL	C-O	7.28	1.32	1.24
1	A	31	SER	CA-CB	7.25	1.64	1.53
1	A	133	LEU	C-N	-7.23	1.20	1.33
1	A	139	MET	CA-CB	7.23	1.62	1.52
1	A	185	ASN	CG-OD1	7.22	1.37	1.23
1	A	76	SER	CA-C	7.20	1.61	1.52
1	A	133	LEU	C-O	7.18	1.32	1.24
1	A	91	ARG	CZ-NH1	7.17	1.42	1.32
1	A	138	ILE	C-N	7.12	1.43	1.33
1	A	33	TYR	CA-C	7.07	1.61	1.52
1	A	48	ASN	C-N	-6.84	1.23	1.33
1	A	91	ARG	NE-CZ	6.80	1.40	1.33
1	A	30	GLU	N-CA	6.75	1.54	1.46
1	A	165	VAL	C-O	6.69	1.31	1.24
1	A	129	GLY	N-CA	6.61	1.54	1.44
1	A	127	HIS	CD2-NE2	6.60	1.45	1.37
1	A	128	PRO	C-O	6.59	1.30	1.23
1	A	152	ASP	CA-C	6.55	1.61	1.52
1	A	91	ARG	CZ-NH2	6.54	1.42	1.33
1	A	53	GLY	C-N	6.53	1.42	1.33
1	A	54	LYS	CA-CB	6.51	1.63	1.53
1	A	121	TYR	N-CA	6.49	1.54	1.46
1	A	56	THR	CA-CB	6.48	1.63	1.53
1	A	24	TRP	CA-CB	6.43	1.62	1.54
1	A	123	GLU	C-O	6.42	1.31	1.24
1	A	116	GLY	C-O	-6.29	1.17	1.23
1	A	169	VAL	N-CA	6.26	1.54	1.46
1	A	92	SER	N-CA	6.22	1.53	1.46
1	A	82	PRO	C-O	6.13	1.31	1.24
1	A	114	ILE	CA-CB	6.03	1.61	1.54
1	A	177	TYR	CA-CB	6.00	1.64	1.53
1	A	70	ARG	C-N	-5.98	1.26	1.33
1	A	130	HIS	N-CA	5.98	1.53	1.46
1	A	126	ASN	CG-OD1	5.91	1.34	1.23
1	A	110	ASP	C-O	5.86	1.31	1.24
1	A	13	ASN	N-CA	5.85	1.52	1.46
1	A	8	VAL	CA-CB	5.85	1.61	1.55
1	A	151	ILE	C-O	5.83	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	PRO	N-CA	5.82	1.55	1.47
1	A	171	GLU	C-O	5.82	1.30	1.23
1	A	135	VAL	CA-CB	5.80	1.61	1.54
1	A	74	VAL	C-O	5.75	1.30	1.24
1	A	162	TYR	CA-CB	5.73	1.63	1.53
1	A	83	PRO	C-O	5.63	1.30	1.23
1	A	145	ASP	C-O	5.62	1.31	1.24
1	A	36	ARG	CZ-NH2	5.60	1.40	1.33
1	A	77	ARG	CD-NE	5.58	1.54	1.46
1	A	141	ASP	C-N	5.56	1.41	1.33
1	A	15	GLY	C-O	5.55	1.30	1.23
1	A	179	PHE	C-O	5.52	1.30	1.24
1	A	155	LYS	C-O	5.51	1.32	1.23
1	A	116	GLY	N-CA	5.51	1.51	1.45
1	A	80	LYS	C-O	5.47	1.31	1.24
1	A	146	THR	CB-OG1	5.35	1.52	1.43
1	A	87	HIS	C-O	5.34	1.30	1.24
1	A	75	LEU	C-N	5.30	1.40	1.33
1	A	24	TRP	CZ2-CH2	5.29	1.47	1.37
1	A	175	ILE	N-CA	5.23	1.52	1.46
1	A	26	PRO	N-CD	5.22	1.55	1.47
1	A	185	ASN	N-CA	5.18	1.53	1.46
1	A	133	LEU	CB-CG	-5.12	1.43	1.53
1	A	132	LYS	N-CA	5.12	1.52	1.46
1	A	40	THR	CA-CB	5.05	1.60	1.53
1	A	96	ALA	N-CA	5.05	1.52	1.46
1	A	25	PRO	N-CA	-5.03	1.39	1.46
1	A	24	TRP	C-N	5.03	1.38	1.33

All (331) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	ASN	OD1-CG-ND2	-21.26	101.34	122.60
1	A	25	PRO	O-C-N	-19.46	112.36	121.31
1	A	25	PRO	CB-CA-C	17.21	127.57	111.39
1	A	120	VAL	O-C-N	14.24	136.71	121.90
1	A	77	ARG	NE-CZ-NH1	-14.09	107.42	121.50
1	A	65	ARG	NE-CZ-NH2	13.50	131.35	119.20
1	A	13	ASN	OD1-CG-ND2	-13.38	109.22	122.60
1	A	35	GLN	OE1-CD-NE2	-12.52	110.08	122.60
1	A	126	ASN	OD1-CG-ND2	-12.51	110.09	122.60
1	A	19	ASN	CB-CG-ND2	12.34	134.91	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	VAL	O-C-N	11.95	136.30	123.03
1	A	44	GLU	CA-C-O	-11.90	107.12	120.69
1	A	9	ALA	CA-C-N	11.77	139.30	122.94
1	A	9	ALA	C-N-CA	11.77	139.30	122.94
1	A	25	PRO	N-CA-CB	-11.71	96.64	103.19
1	A	27	LEU	CA-C-O	-11.60	107.48	120.70
1	A	33	TYR	O-C-N	11.57	134.39	122.12
1	A	44	GLU	O-C-N	11.45	136.44	123.04
1	A	175	ILE	O-C-N	11.45	134.81	123.14
1	A	87	HIS	CE1-NE2-CD2	11.33	120.33	109.00
1	A	72	ASN	OD1-CG-ND2	-11.26	111.34	122.60
1	A	77	ARG	NE-CZ-NH2	11.24	129.32	119.20
1	A	32	ARG	O-C-N	-11.12	110.62	122.07
1	A	70	ARG	CA-C-O	-10.96	108.73	121.11
1	A	181	VAL	O-C-N	-10.95	111.79	123.18
1	A	142	PHE	CA-CB-CG	10.86	124.66	113.80
1	A	25	PRO	CA-C-O	10.73	128.63	120.90
1	A	53	GLY	CA-C-O	10.73	136.69	122.31
1	A	128	PRO	CA-C-O	10.67	135.10	121.98
1	A	126	ASN	CA-C-N	10.42	134.87	120.39
1	A	126	ASN	C-N-CA	10.42	134.87	120.39
1	A	87	HIS	ND1-CE1-NE2	-10.27	98.13	108.40
1	A	77	ARG	CG-CD-NE	-10.25	89.44	112.00
1	A	58	PHE	CA-C-O	-10.24	106.78	119.38
1	A	25	PRO	CA-C-N	10.01	130.64	119.83
1	A	25	PRO	C-N-CA	10.01	130.64	119.83
1	A	24	TRP	CA-C-N	9.99	126.96	119.66
1	A	24	TRP	C-N-CA	9.99	126.96	119.66
1	A	116	GLY	CA-C-O	-9.96	112.40	122.26
1	A	13	ASN	CA-CB-CG	9.91	122.51	112.60
1	A	128	PRO	CB-CA-C	9.89	125.98	110.25
1	A	123	GLU	CA-CB-CG	9.89	133.88	114.10
1	A	126	ASN	CB-CG-OD1	9.86	140.52	120.80
1	A	78	GLU	OE1-CD-OE2	-9.82	99.32	122.90
1	A	9	ALA	O-C-N	-9.79	111.74	123.29
1	A	140	GLN	O-C-N	9.75	133.11	123.46
1	A	146	THR	CA-C-O	-9.67	109.54	120.66
1	A	42	SER	CA-C-O	-9.63	107.53	119.38
1	A	25	PRO	N-CA-C	-9.60	101.26	110.47
1	A	148	PHE	CA-C-N	9.55	129.61	119.78
1	A	148	PHE	C-N-CA	9.55	129.61	119.78
1	A	138	ILE	CB-CG1-CD1	9.52	133.79	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	GLU	O-C-N	9.51	135.13	123.44
1	A	31	SER	N-CA-CB	9.50	124.09	110.12
1	A	138	ILE	CA-C-O	9.38	131.62	120.65
1	A	175	ILE	CA-C-N	-9.36	106.73	122.64
1	A	175	ILE	C-N-CA	-9.36	106.73	122.64
1	A	56	THR	CA-CB-OG1	-9.35	95.57	109.60
1	A	114	ILE	O-C-N	-9.31	112.40	122.83
1	A	18	LYS	O-C-N	-9.24	111.45	123.28
1	A	32	ARG	CA-C-N	9.13	132.51	120.28
1	A	32	ARG	C-N-CA	9.13	132.51	120.28
1	A	148	PHE	CA-CB-CG	-9.10	104.70	113.80
1	A	185	ASN	N-CA-CB	9.08	124.84	110.86
1	A	101	GLU	CB-CG-CD	9.08	128.03	112.60
1	A	138	ILE	CA-CB-CG1	9.07	125.82	110.40
1	A	145	ASP	CB-CG-OD1	9.02	139.14	118.40
1	A	158	LEU	CA-C-O	-8.93	110.54	120.81
1	A	185	ASN	OD1-CG-ND2	-8.82	113.78	122.60
1	A	77	ARG	CD-NE-CZ	-8.77	112.13	124.40
1	A	72	ASN	CA-C-O	-8.76	110.99	120.36
1	A	173	LYS	CB-CA-C	-8.74	97.94	111.66
1	A	140	GLN	N-CA-CB	8.69	124.77	111.56
1	A	10	VAL	CA-CB-CG2	8.64	125.08	110.40
1	A	123	GLU	CA-C-O	-8.64	111.80	120.70
1	A	85	GLY	CA-C-N	8.63	133.12	120.87
1	A	85	GLY	C-N-CA	8.63	133.12	120.87
1	A	65	ARG	CA-C-O	-8.54	110.04	119.61
1	A	171	GLU	CA-C-N	-8.53	106.93	121.94
1	A	171	GLU	C-N-CA	-8.53	106.93	121.94
1	A	110	ASP	O-C-N	-8.53	111.25	122.59
1	A	108	LYS	N-CA-C	8.46	123.99	112.90
1	A	35	GLN	CA-C-O	8.42	129.66	120.82
1	A	130	HIS	CA-C-O	-8.35	111.17	120.69
1	A	184	LYS	CB-CA-C	-8.35	93.47	109.66
1	A	101	GLU	CA-CB-CG	8.31	130.72	114.10
1	A	145	ASP	OD1-CG-OD2	-8.31	102.96	122.90
1	A	30	GLU	N-CA-C	-8.31	102.18	111.07
1	A	95	ASP	O-C-N	8.28	131.59	122.15
1	A	19	ASN	CA-C-O	-8.27	112.25	121.84
1	A	119	SER	O-C-N	-8.19	113.44	122.12
1	A	52	MET	CA-C-O	-8.12	111.64	121.06
1	A	28	ARG	N-CA-CB	8.11	122.71	110.22
1	A	172	GLU	CB-CA-C	8.06	125.64	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	VAL	CA-C-O	8.04	128.39	120.27
1	A	126	ASN	CA-CB-CG	8.00	120.60	112.60
1	A	31	SER	CA-CB-OG	-8.00	95.10	111.10
1	A	33	TYR	CA-C-N	-7.99	109.57	120.28
1	A	33	TYR	C-N-CA	-7.99	109.57	120.28
1	A	133	LEU	CA-C-O	-7.98	111.74	120.43
1	A	174	GLY	CA-C-N	-7.95	112.84	123.10
1	A	174	GLY	C-N-CA	-7.95	112.84	123.10
1	A	53	GLY	N-CA-C	-7.91	102.41	112.54
1	A	48	ASN	OD1-CG-ND2	7.88	130.48	122.60
1	A	90	SER	N-CA-CB	7.84	125.63	111.37
1	A	135	VAL	CA-C-O	-7.78	112.20	120.53
1	A	130	HIS	CA-CB-CG	-7.78	106.02	113.80
1	A	119	SER	N-CA-CB	-7.76	98.71	110.12
1	A	172	GLU	CB-CG-CD	7.76	125.79	112.60
1	A	65	ARG	NH1-CZ-NH2	-7.71	109.28	119.30
1	A	174	GLY	O-C-N	7.70	131.73	122.34
1	A	58	PHE	O-C-N	7.68	132.72	122.43
1	A	50	VAL	N-CA-CB	7.68	121.13	111.46
1	A	115	VAL	O-C-N	7.67	130.10	122.05
1	A	102	GLN	N-CA-C	-7.65	100.16	109.72
1	A	129	GLY	O-C-N	7.63	134.30	122.70
1	A	185	ASN	CA-CB-CG	7.58	120.17	112.60
1	A	53	GLY	O-C-N	-7.57	111.48	122.69
1	A	44	GLU	CA-CB-CG	7.57	129.24	114.10
1	A	108	LYS	CB-CA-C	-7.56	94.48	109.67
1	A	129	GLY	CA-C-O	-7.51	115.22	121.76
1	A	52	MET	O-C-N	7.50	131.97	123.27
1	A	31	SER	CB-CA-C	-7.49	98.35	110.79
1	A	44	GLU	CB-CA-C	-7.49	97.63	109.84
1	A	72	ASN	CB-CG-ND2	7.48	127.63	116.40
1	A	138	ILE	N-CA-C	-7.47	96.80	108.23
1	A	167	SER	CA-CB-OG	-7.47	96.16	111.10
1	A	165	VAL	CG1-CB-CG2	7.46	127.22	110.80
1	A	81	GLU	CA-CB-CG	7.43	128.97	114.10
1	A	166	LEU	O-C-N	-7.41	113.77	122.95
1	A	183	GLU	CA-C-O	7.36	128.49	120.32
1	A	134	PHE	N-CA-CB	7.36	122.90	110.46
1	A	119	SER	CA-C-N	7.31	129.92	120.56
1	A	119	SER	C-N-CA	7.31	129.92	120.56
1	A	123	GLU	N-CA-CB	-7.30	99.48	110.07
1	A	6	CYS	N-CA-CB	7.29	123.52	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	GLY	CA-C-O	-7.29	111.69	119.27
1	A	126	ASN	O-C-N	-7.29	112.87	122.42
1	A	100	THR	CA-CB-OG1	-7.22	98.76	109.60
1	A	74	VAL	O-C-N	-7.17	115.82	123.14
1	A	161	GLU	CB-CG-CD	7.17	124.79	112.60
1	A	74	VAL	CA-C-N	7.14	132.57	122.72
1	A	74	VAL	C-N-CA	7.14	132.57	122.72
1	A	24	TRP	CB-CA-C	7.12	119.97	109.08
1	A	89	LEU	CA-C-O	-7.09	112.44	120.32
1	A	109	VAL	CA-C-O	-7.05	113.02	120.57
1	A	76	SER	CA-C-N	-7.04	110.08	122.26
1	A	76	SER	C-N-CA	-7.04	110.08	122.26
1	A	164	GLY	O-C-N	-7.03	113.63	122.41
1	A	133	LEU	CA-C-N	6.99	133.49	123.14
1	A	133	LEU	C-N-CA	6.99	133.49	123.14
1	A	162	TYR	CA-C-N	6.97	128.07	119.98
1	A	162	TYR	C-N-CA	6.97	128.07	119.98
1	A	56	THR	O-C-N	-6.95	114.76	122.12
1	A	179	PHE	CA-C-O	-6.93	112.67	120.43
1	A	146	THR	O-C-N	6.89	131.68	123.27
1	A	137	ARG	N-CA-CB	6.86	120.92	109.94
1	A	30	GLU	CA-C-O	-6.85	113.62	120.82
1	A	77	ARG	CA-CB-CG	-6.85	100.40	114.10
1	A	126	ASN	CB-CA-C	6.84	121.55	109.65
1	A	34	PHE	CA-CB-CG	-6.81	106.99	113.80
1	A	179	PHE	O-C-N	-6.79	115.33	123.13
1	A	13	ASN	CA-C-N	6.75	132.19	122.40
1	A	13	ASN	C-N-CA	6.75	132.19	122.40
1	A	17	GLY	N-CA-C	-6.75	99.00	111.14
1	A	45	GLY	N-CA-C	-6.66	106.04	115.30
1	A	175	ILE	CA-C-O	-6.65	113.14	120.72
1	A	134	PHE	CA-CB-CG	-6.64	107.16	113.80
1	A	170	GLN	OE1-CD-NE2	-6.63	115.97	122.60
1	A	9	ALA	CA-C-O	-6.62	113.17	120.38
1	A	78	GLU	CA-CB-CG	6.60	127.30	114.10
1	A	11	SER	CA-C-O	6.60	129.53	121.94
1	A	84	GLN	CB-CG-CD	6.59	123.80	112.60
1	A	95	ASP	CA-C-O	-6.58	113.44	120.42
1	A	54	LYS	N-CA-C	6.51	118.38	111.28
1	A	147	PHE	CA-CB-CG	-6.51	107.29	113.80
1	A	113	TRP	CZ3-CH2-CZ2	6.50	129.95	121.50
1	A	99	LEU	N-CA-C	6.46	119.31	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	PRO	CA-C-N	-6.46	107.83	123.46
1	A	128	PRO	C-N-CA	-6.46	107.83	123.46
1	A	57	TRP	CA-C-N	6.43	131.46	120.72
1	A	57	TRP	C-N-CA	6.43	131.46	120.72
1	A	170	GLN	O-C-N	6.43	130.30	122.84
1	A	113	TRP	CA-C-O	-6.43	113.58	120.46
1	A	19	ASN	N-CA-C	6.37	120.18	111.39
1	A	74	VAL	CA-CB-CG2	6.37	121.23	110.40
1	A	101	GLU	CB-CA-C	-6.36	99.04	110.37
1	A	157	LYS	CG-CD-CE	6.35	125.91	111.30
1	A	151	ILE	O-C-N	6.28	130.61	122.94
1	A	54	LYS	N-CA-CB	-6.27	100.90	110.12
1	A	157	LYS	CA-CB-CG	-6.25	101.59	114.10
1	A	29	ASN	CA-CB-CG	6.24	118.83	112.60
1	A	142	PHE	N-CA-CB	6.24	121.29	110.81
1	A	75	LEU	N-CA-CB	6.23	120.59	110.43
1	A	172	GLU	O-C-N	-6.23	116.12	123.41
1	A	176	LYS	O-C-N	6.20	130.23	123.10
1	A	19	ASN	O-C-N	6.19	130.22	122.55
1	A	69	GLY	CA-C-N	6.18	132.52	122.81
1	A	69	GLY	C-N-CA	6.18	132.52	122.81
1	A	91	ARG	CA-CB-CG	-6.17	101.75	114.10
1	A	43	VAL	O-C-N	-6.17	116.34	122.76
1	A	115	VAL	CA-C-O	-6.17	113.81	119.91
1	A	127	HIS	CA-C-O	6.17	126.58	120.17
1	A	32	ARG	CD-NE-CZ	6.16	133.03	124.40
1	A	12	GLN	OE1-CD-NE2	6.16	128.76	122.60
1	A	127	HIS	N-CA-C	-6.14	101.84	109.64
1	A	65	ARG	CD-NE-CZ	6.11	132.96	124.40
1	A	86	ALA	N-CA-CB	6.10	118.93	109.97
1	A	46	LYS	CA-C-N	6.09	132.37	122.81
1	A	46	LYS	C-N-CA	6.09	132.37	122.81
1	A	147	PHE	CA-C-N	6.09	129.13	120.49
1	A	147	PHE	C-N-CA	6.09	129.13	120.49
1	A	171	GLU	OE1-CD-OE2	6.05	137.43	122.90
1	A	13	ASN	CB-CG-OD1	6.05	132.91	120.80
1	A	98	LYS	CA-C-N	6.04	129.50	120.31
1	A	98	LYS	C-N-CA	6.04	129.50	120.31
1	A	64	ASN	CA-C-O	-6.04	112.49	119.56
1	A	44	GLU	N-CA-C	6.00	119.30	109.76
1	A	40	THR	CA-CB-OG1	-5.99	100.61	109.60
1	A	138	ILE	N-CA-CB	5.99	117.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	LYS	CG-CD-CE	-5.96	97.59	111.30
1	A	119	SER	CA-C-O	5.96	126.86	120.55
1	A	136	THR	O-C-N	-5.94	115.80	122.93
1	A	141	ASP	CB-CG-OD2	5.93	132.03	118.40
1	A	166	LEU	CA-C-O	5.90	127.65	120.92
1	A	1	VAL	N-CA-CB	-5.90	101.47	111.50
1	A	48	ASN	O-C-N	5.90	129.67	123.06
1	A	88	PHE	CA-C-O	-5.87	114.77	121.40
1	A	141	ASP	CA-CB-CG	-5.87	106.73	112.60
1	A	122	LYS	CA-C-N	5.84	128.39	120.44
1	A	122	LYS	C-N-CA	5.84	128.39	120.44
1	A	176	LYS	CA-C-O	-5.80	114.43	121.28
1	A	36	ARG	CG-CD-NE	5.80	124.76	112.00
1	A	163	PRO	N-CA-CB	5.80	108.33	103.17
1	A	26	PRO	N-CA-CB	5.79	108.48	103.27
1	A	137	ARG	O-C-N	-5.77	115.32	122.82
1	A	47	GLN	CB-CG-CD	-5.77	102.79	112.60
1	A	91	ARG	CG-CD-NE	-5.77	99.31	112.00
1	A	8	VAL	CB-CA-C	-5.75	103.81	111.80
1	A	172	GLU	CG-CD-OE2	-5.71	105.26	118.40
1	A	121	TYR	CZ-CE2-CD2	-5.71	109.32	119.60
1	A	167	SER	CA-C-N	-5.69	110.64	122.07
1	A	167	SER	C-N-CA	-5.69	110.64	122.07
1	A	109	VAL	N-CA-C	5.67	116.47	108.36
1	A	72	ASN	O-C-N	5.65	129.66	123.22
1	A	113	TRP	CE3-CZ3-CH2	-5.64	113.77	121.10
1	A	27	LEU	O-C-N	5.62	130.32	123.01
1	A	76	SER	CB-CA-C	-5.62	100.67	109.72
1	A	81	GLU	O-C-N	5.59	125.73	121.65
1	A	168	ASP	O-C-N	5.58	129.19	122.94
1	A	11	SER	O-C-N	-5.57	115.79	122.65
1	A	120	VAL	CA-C-N	-5.56	113.21	120.44
1	A	120	VAL	C-N-CA	-5.56	113.21	120.44
1	A	113	TRP	CA-C-N	5.56	129.58	121.80
1	A	113	TRP	C-N-CA	5.56	129.58	121.80
1	A	112	VAL	CA-CB-CG1	-5.56	100.95	110.40
1	A	75	LEU	CA-C-O	5.56	126.49	120.43
1	A	33	TYR	CA-C-O	-5.55	114.67	120.55
1	A	47	GLN	CA-CB-CG	-5.53	103.03	114.10
1	A	125	MET	CA-CB-CG	-5.53	103.04	114.10
1	A	154	GLU	CG-CD-OE2	-5.53	105.69	118.40
1	A	16	ILE	CB-CA-C	5.50	116.04	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	LYS	CA-C-N	5.50	128.65	120.95
1	A	157	LYS	C-N-CA	5.50	128.65	120.95
1	A	162	TYR	CA-C-O	5.48	125.31	119.50
1	A	12	GLN	CA-CB-CG	-5.45	103.19	114.10
1	A	48	ASN	CA-C-O	-5.44	114.83	121.36
1	A	111	MET	CA-CB-CG	-5.43	103.23	114.10
1	A	143	GLU	N-CA-CB	-5.43	101.39	109.69
1	A	101	GLU	CG-CD-OE1	5.41	130.84	118.40
1	A	22	LEU	CB-CG-CD1	5.40	126.89	110.70
1	A	151	ILE	N-CA-CB	5.40	117.15	111.00
1	A	11	SER	N-CA-C	-5.39	103.58	110.53
1	A	9	ALA	N-CA-CB	5.38	119.02	110.57
1	A	95	ASP	CA-C-N	-5.38	112.64	120.29
1	A	95	ASP	C-N-CA	-5.38	112.64	120.29
1	A	78	GLU	CG-CD-OE1	5.37	130.75	118.40
1	A	150	GLU	CA-C-O	5.37	127.10	121.19
1	A	118	SER	N-CA-C	5.36	120.21	111.37
1	A	138	ILE	CA-C-N	-5.34	114.07	122.08
1	A	138	ILE	C-N-CA	-5.34	114.07	122.08
1	A	44	GLU	CG-CD-OE2	-5.34	106.12	118.40
1	A	92	SER	CA-C-N	-5.34	112.20	120.31
1	A	92	SER	C-N-CA	-5.34	112.20	120.31
1	A	109	VAL	CA-CB-CG2	5.34	119.47	110.40
1	A	56	THR	CA-C-O	5.33	126.20	120.55
1	A	40	THR	N-CA-C	5.33	117.42	109.59
1	A	179	PHE	CA-C-N	5.32	131.17	122.81
1	A	179	PHE	C-N-CA	5.32	131.17	122.81
1	A	71	ILE	N-CA-CB	5.31	116.90	110.95
1	A	78	GLU	CB-CG-CD	5.31	121.63	112.60
1	A	16	ILE	CA-CB-CG2	5.31	119.52	110.50
1	A	105	LEU	N-CA-C	5.30	119.80	113.23
1	A	121	TYR	CB-CG-CD2	-5.29	112.86	120.80
1	A	86	ALA	CA-C-O	5.29	127.08	121.16
1	A	113	TRP	CH2-CZ2-CE2	-5.28	110.63	117.50
1	A	47	GLN	CB-CA-C	-5.27	98.95	109.33
1	A	32	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	A	183	GLU	CG-CD-OE2	5.25	130.47	118.40
1	A	141	ASP	CB-CG-OD1	-5.24	106.34	118.40
1	A	7	ILE	CA-C-O	-5.24	114.72	120.43
1	A	22	LEU	CA-C-N	5.20	124.82	119.56
1	A	22	LEU	C-N-CA	5.20	124.82	119.56
1	A	16	ILE	CA-CB-CG1	-5.20	101.56	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	HIS	CG-CD2-NE2	-5.20	102.00	107.20
1	A	66	PRO	N-CD-CG	-5.19	97.57	103.80
1	A	182	TYR	N-CA-CB	5.18	119.04	110.69
1	A	137	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	A	12	GLN	CB-CG-CD	5.14	121.34	112.60
1	A	110	ASP	CB-CG-OD2	5.14	130.23	118.40
1	A	32	ARG	CA-C-O	5.14	126.22	120.82
1	A	168	ASP	N-CA-C	5.14	118.12	110.52
1	A	54	LYS	CD-CE-NZ	5.13	128.33	111.90
1	A	121	TYR	CE1-CZ-CE2	5.13	130.57	120.30
1	A	9	ALA	CB-CA-C	5.13	118.59	109.72
1	A	70	ARG	CA-CB-CG	-5.13	103.85	114.10
1	A	50	VAL	CB-CA-C	5.12	118.44	110.96
1	A	114	ILE	CB-CA-C	5.12	117.07	111.08
1	A	58	PHE	CA-CB-CG	-5.10	108.70	113.80
1	A	184	LYS	CA-CB-CG	5.09	124.28	114.10
1	A	14	MET	CA-C-O	-5.08	114.51	120.81
1	A	133	LEU	CA-CB-CG	5.08	134.09	116.30
1	A	159	LEU	CA-C-O	5.08	125.17	120.60
1	A	87	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	A	179	PHE	N-CA-C	5.06	117.01	108.96
1	A	118	SER	CA-C-O	5.04	126.57	120.92
1	A	80	LYS	CA-C-O	5.04	125.73	119.79
1	A	36	ARG	CA-C-O	-5.03	115.09	120.42
1	A	176	LYS	CB-CG-CD	-5.01	99.77	111.30
1	A	57	TRP	O-C-N	-5.01	116.88	122.09
1	A	148	PHE	O-C-N	-5.01	115.82	121.43

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	TYR	Sidechain
1	A	65	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	1497	0	1506	55	0
2	A	48	0	26	2	0
3	A	32	0	20	2	0
4	A	51	0	0	3	0
All	All	1628	0	1552	55	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 18.

All (55) 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:28:ARG:HD3	1:A:32:ARG:NH2	1.63	1.14
1:A:28:ARG:CD	1:A:32:ARG:HH21	1.75	0.99
1:A:28:ARG:CZ	1:A:32:ARG:HH21	1.79	0.95
1:A:125:MET:HE2	1:A:133:LEU:HD21	1.50	0.93
1:A:28:ARG:HG3	4:A:203:HOH:O	1.66	0.93
1:A:28:ARG:NE	1:A:32:ARG:HH21	1.67	0.91
1:A:28:ARG:CD	1:A:32:ARG:NH2	2.33	0.90
1:A:114:ILE:HD13	1:A:124:ALA:HB2	1.57	0.85
1:A:28:ARG:HD3	1:A:32:ARG:HH21	1.34	0.83
1:A:125:MET:HE2	1:A:133:LEU:CD2	2.09	0.81
1:A:72:ASN:H	1:A:87:HIS:HD2	1.30	0.77
1:A:114:ILE:HD13	1:A:124:ALA:CB	2.16	0.76
1:A:12:GLN:HB3	1:A:141:ASP:OD1	1.85	0.75
1:A:36:ARG:NH1	1:A:37:MET:HE3	2.01	0.75
1:A:125:MET:HE1	1:A:148:PHE:CZ	2.23	0.74
1:A:37:MET:HA	1:A:37:MET:HE2	1.71	0.72
1:A:125:MET:HE1	1:A:148:PHE:HZ	1.54	0.71
1:A:42:SER:OG	1:A:110:ASP:OD2	2.07	0.71
1:A:35:GLN:NE2	3:A:188:MOT:HG2	2.07	0.69
1:A:35:GLN:HE21	3:A:188:MOT:HG2	1.59	0.68
1:A:168:ASP:OD1	1:A:170:GLN:NE2	2.26	0.68
1:A:125:MET:CE	1:A:148:PHE:HZ	2.11	0.64
1:A:28:ARG:CZ	1:A:32:ARG:NH2	2.56	0.64
1:A:10:VAL:HG22	1:A:14:MET:HA	1.80	0.63
1:A:36:ARG:NH1	1:A:37:MET:CE	2.61	0.63
1:A:95:ASP:HA	1:A:98:LYS:HE3	1.80	0.63
1:A:28:ARG:NE	1:A:32:ARG:NH2	2.45	0.62
1:A:130:HIS:HE1	1:A:183:GLU:HG3	1.64	0.62
1:A:130:HIS:HE1	1:A:183:GLU:CG	2.13	0.61
1:A:72:ASN:H	1:A:87:HIS:CD2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:TYR:CZ	1:A:184:LYS:HD3	2.39	0.58
1:A:130:HIS:CE1	1:A:183:GLU:HG3	2.38	0.58
1:A:130:HIS:ND1	1:A:184:LYS:O	2.39	0.55
1:A:10:VAL:CG2	1:A:14:MET:HA	2.36	0.55
1:A:28:ARG:CG	4:A:203:HOH:O	2.39	0.54
1:A:125:MET:CE	1:A:148:PHE:CZ	2.91	0.51
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.94	0.49
1:A:28:ARG:NH1	1:A:32:ARG:HH21	2.10	0.49
1:A:140:GLN:HG3	1:A:142:PHE:CE2	2.49	0.47
1:A:25:PRO:HA	1:A:26:PRO:HD3	1.82	0.47
1:A:152:ASP:OD2	1:A:155:LYS:HE2	2.15	0.47
1:A:40:THR:O	1:A:111:MET:CE	2.63	0.46
1:A:47:GLN:HG2	1:A:69:GLY:O	2.17	0.45
1:A:1:VAL:HG23	1:A:2:GLY:N	2.32	0.44
1:A:75:LEU:O	2:A:187:NDP:H1B	2.18	0.43
1:A:94:ASP:O	1:A:98:LYS:HB2	2.19	0.43
1:A:24:TRP:CB	1:A:25:PRO:HD2	2.48	0.42
1:A:28:ARG:O	1:A:28:ARG:HG2	2.18	0.42
1:A:36:ARG:CZ	1:A:37:MET:HE3	2.48	0.42
1:A:130:HIS:NE2	1:A:183:GLU:OE2	2.52	0.42
1:A:1:VAL:HG21	1:A:109:VAL:O	2.20	0.42
1:A:16:ILE:O	2:A:187:NDP:H2N	2.20	0.42
1:A:166:LEU:O	4:A:199:HOH:O	2.21	0.41
1:A:186:ASP:OD1	1:A:186:ASP:C	2.64	0.41
1:A:133:LEU:HB2	1:A:182:TYR:HB2	2.04	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%)	180 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	153 (91%)	15 (9%)	9 6

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	22	LEU
1	A	63	LYS
1	A	68	LYS
1	A	72	ASN
1	A	98	LYS
1	A	99	LEU
1	A	104	GLU
1	A	115	VAL
1	A	119	SER
1	A	131	LEU
1	A	133	LEU
1	A	140	GLN
1	A	167	SER
1	A	185	ASN

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	19	ASN
1	A	35	GLN
1	A	87	HIS
1	A	127	HIS
1	A	140	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	3.50	13 (38%)	41,48,48	3.48	21 (51%)
2	NDP	A	187	-	51,52,52	3.05	27 (52%)	71,80,80	2.87	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	-	-	0/25/25/25	0/3/3/3
2	NDP	A	187	-	-	10/34/77/77	0/5/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	188	MOT	O8-C8A	-9.30	1.25	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	P2B-O2B	8.45	1.74	1.59
2	A	187	NDP	PN-O3	8.18	1.68	1.59
3	A	188	MOT	C11-C	-7.76	1.33	1.50
3	A	188	MOT	C4A-C4	-7.24	1.34	1.42
3	A	188	MOT	C9-N10	7.14	1.57	1.46
2	A	187	NDP	O4B-C4B	-6.86	1.29	1.45
3	A	188	MOT	C2-N3	-6.16	1.24	1.35
3	A	188	MOT	C2-NA2	5.58	1.45	1.33
2	A	187	NDP	C5A-C6A	5.54	1.56	1.41
3	A	188	MOT	C9-C6	4.83	1.56	1.51
2	A	187	NDP	O3B-C3B	4.50	1.54	1.43
2	A	187	NDP	C5A-C4A	-4.49	1.31	1.39
2	A	187	NDP	C3B-C4B	4.35	1.64	1.53
2	A	187	NDP	C4A-N3A	4.28	1.42	1.34
2	A	187	NDP	O4D-C1D	3.70	1.50	1.42
2	A	187	NDP	C2B-C1B	3.55	1.61	1.53
2	A	187	NDP	C5A-N7A	3.54	1.45	1.39
3	A	188	MOT	CM-N10	3.52	1.51	1.46
2	A	187	NDP	C3D-C4D	3.49	1.61	1.53
3	A	188	MOT	C8A-N1	3.33	1.37	1.32
2	A	187	NDP	PN-O2N	-3.18	1.40	1.55
2	A	187	NDP	PA-O2A	-3.14	1.40	1.55
3	A	188	MOT	C13-C14	-3.09	1.33	1.39
2	A	187	NDP	O4D-C4D	3.00	1.51	1.45
2	A	187	NDP	C4A-N9A	-2.97	1.31	1.37
2	A	187	NDP	C6N-N1N	2.94	1.44	1.37
2	A	187	NDP	C7N-C3N	2.81	1.54	1.48
3	A	188	MOT	C4-NA4	-2.78	1.27	1.34
2	A	187	NDP	C3B-C2B	2.44	1.58	1.53
3	A	188	MOT	C7-C6	-2.42	1.32	1.34
2	A	187	NDP	C5D-C4D	2.37	1.58	1.51
2	A	187	NDP	PA-O5B	2.31	1.68	1.59
2	A	187	NDP	PN-O1N	-2.29	1.42	1.50
2	A	187	NDP	C5B-C4B	2.17	1.58	1.51
2	A	187	NDP	P2B-O2X	-2.16	1.46	1.54
2	A	187	NDP	C1D-N1N	2.16	1.52	1.46
3	A	188	MOT	O8-C7	-2.07	1.32	1.38
2	A	187	NDP	P2B-O3X	-2.03	1.47	1.54
2	A	187	NDP	C1B-N9A	-2.02	1.40	1.46

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188	MOT	O8-C8A-C4A	12.50	118.07	110.00
2	A	187	NDP	C6N-N1N-C2N	8.14	128.03	119.32
2	A	187	NDP	O7N-C7N-C3N	-7.04	107.64	120.90
2	A	187	NDP	C3N-C2N-N1N	-6.51	113.64	123.20
3	A	188	MOT	C13-C14-N10	6.22	130.26	121.59
2	A	187	NDP	C5A-C4A-N9A	5.59	111.90	105.81
3	A	188	MOT	CB-CA-N	-5.57	99.88	110.91
3	A	188	MOT	NA2-C2-N1	-5.57	108.88	117.22
2	A	187	NDP	C1D-N1N-C2N	-5.40	112.25	121.14
2	A	187	NDP	PN-O5D-C5D	5.37	152.10	121.35
3	A	188	MOT	C16-C15-C14	5.22	126.91	120.30
3	A	188	MOT	C12-C13-C14	4.88	126.47	120.30
3	A	188	MOT	C15-C14-C13	-4.78	110.05	119.18
2	A	187	NDP	O3D-C3D-C2D	4.75	127.04	111.82
3	A	188	MOT	C2-N1-C8A	-4.58	109.60	115.96
2	A	187	NDP	P2B-O2B-C2B	-4.52	111.35	123.43
2	A	187	NDP	C4A-C5A-N7A	-4.32	105.64	110.58
2	A	187	NDP	O3X-P2B-O1X	4.15	126.99	110.83
2	A	187	NDP	O3D-C3D-C4D	-4.05	99.46	111.08
2	A	187	NDP	O2N-PN-O3	-3.98	96.52	107.27
2	A	187	NDP	C6A-C5A-N7A	3.95	139.71	132.09
2	A	187	NDP	C4B-O4B-C1B	3.93	118.14	109.47
3	A	188	MOT	CM-N10-C9	-3.92	104.70	114.49
2	A	187	NDP	O4D-C1D-N1N	-3.89	100.67	108.08
2	A	187	NDP	C5B-C4B-C3B	-3.53	102.51	115.21
2	A	187	NDP	N3A-C4A-N9A	-3.40	121.39	127.17
3	A	188	MOT	O2-CT-CA	3.37	124.91	113.51
2	A	187	NDP	O3-PA-O1A	-3.30	100.79	110.70
2	A	187	NDP	O2X-P2B-O2B	-3.23	93.27	105.85
2	A	187	NDP	C2D-C1D-N1N	3.22	121.23	113.31
3	A	188	MOT	CM-N10-C14	3.18	124.86	119.59
3	A	188	MOT	CB-CA-CT	-3.13	102.92	110.35
3	A	188	MOT	C16-C11-C12	-3.08	114.65	118.57
3	A	188	MOT	O2-CT-O1	-3.07	117.11	124.08
3	A	188	MOT	C4A-C6-C7	3.06	107.93	105.34
3	A	188	MOT	N3-C2-N1	2.97	130.04	125.48
2	A	187	NDP	O2A-PA-O1A	2.82	125.55	112.44
2	A	187	NDP	O2B-C2B-C1B	-2.74	100.42	110.05
2	A	187	NDP	C3N-C7N-N7N	2.72	122.49	117.67
2	A	187	NDP	O5B-C5B-C4B	-2.70	99.79	108.99
2	A	187	NDP	O4B-C1B-C2B	-2.70	101.95	106.59
2	A	187	NDP	O5D-PN-O1N	2.66	119.49	108.94
2	A	187	NDP	O7N-C7N-N7N	2.66	128.87	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	187	NDP	C3B-C2B-C1B	-2.63	97.77	102.81
2	A	187	NDP	C5D-C4D-C3D	-2.58	105.91	115.21
2	A	187	NDP	O3-PN-O1N	2.54	118.36	110.70
3	A	188	MOT	NA2-C2-N3	2.51	120.99	117.22
2	A	187	NDP	N9A-C8A-N7A	-2.49	110.41	113.94
3	A	188	MOT	OE2-CD-OE1	2.32	129.30	123.33
3	A	188	MOT	OE2-CD-CG	-2.31	106.71	114.00
3	A	188	MOT	C16-C11-C	2.26	127.92	120.60
2	A	187	NDP	O5D-C5D-C4D	-2.16	101.64	108.99
3	A	188	MOT	O8-C8A-N1	-2.03	118.13	119.20

There are no chirality outliers.

All (10) 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
2	A	187	NDP	O4D-C1D-N1N-C2N
2	A	187	NDP	C2D-C1D-N1N-C2N
2	A	187	NDP	PN-O3-PA-O1A
2	A	187	NDP	PA-O3-PN-O2N

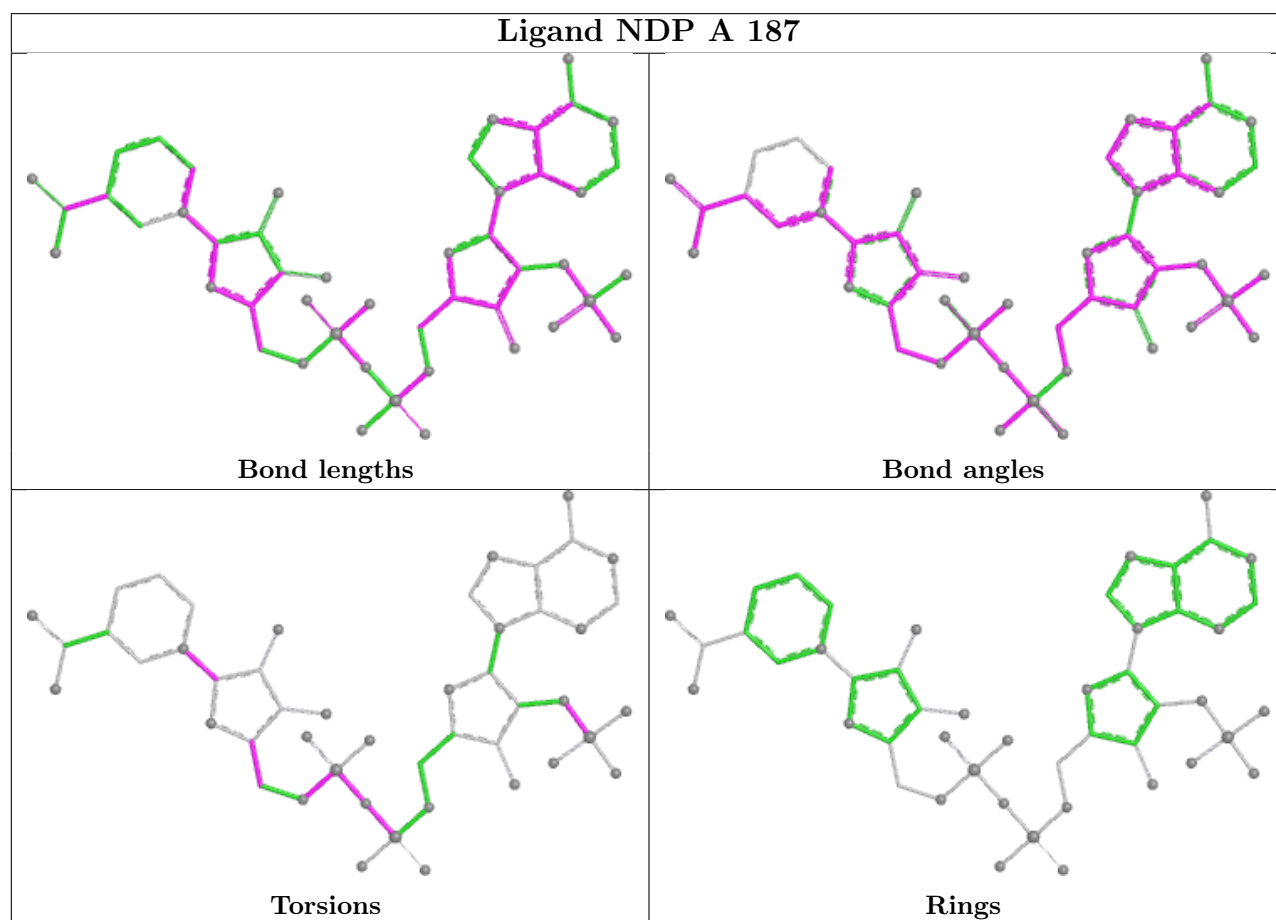
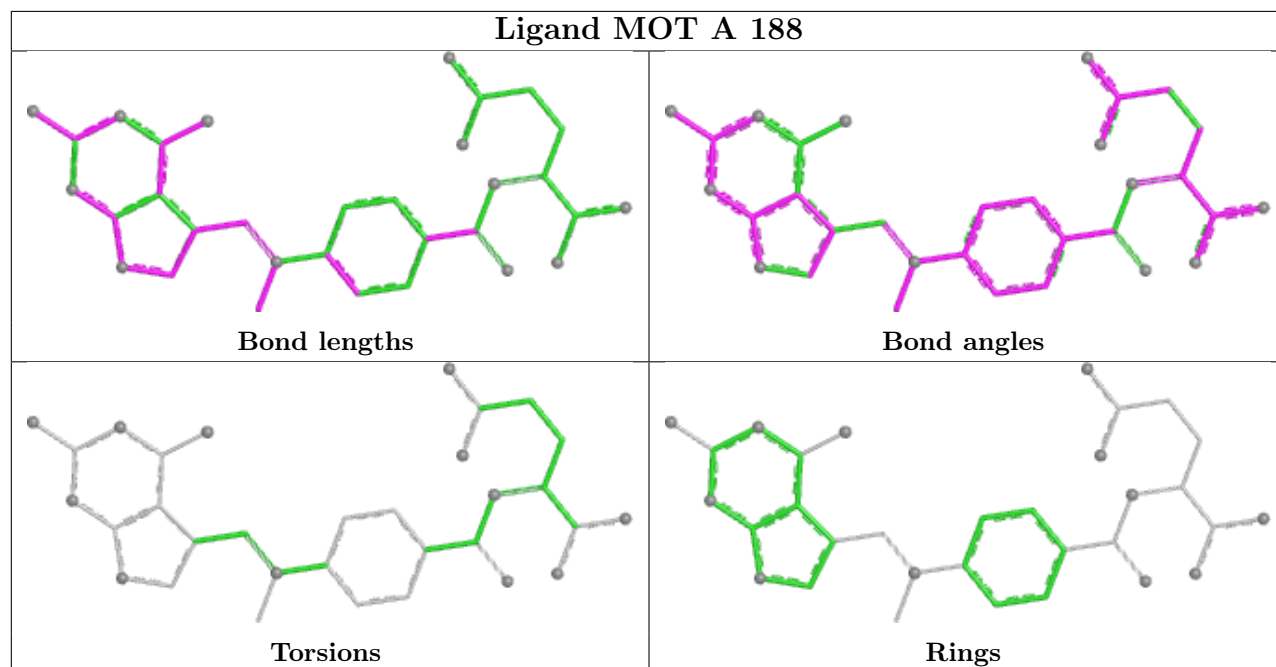
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	188	MOT	2	0
2	A	187	NDP	2	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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.