



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:36 PM UTC

PDB ID : 1OHJ / pdb_00001ohj
Title : HUMAN DIHYDROFOLATE REDUCTASE, MONOCLINIC (P21) CRYSTAL FORM
Authors : Cody, V.; Galitsky, N.; Luft, J.R.; Pangborn, W.
Deposited on : 1997-09-17
Resolution : 2.50 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

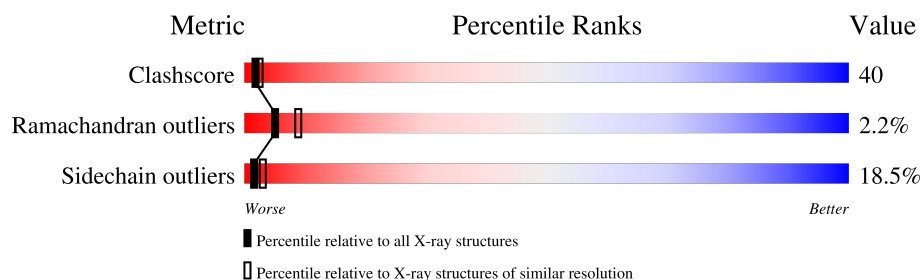
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	186	

2 Entry composition [i](#)

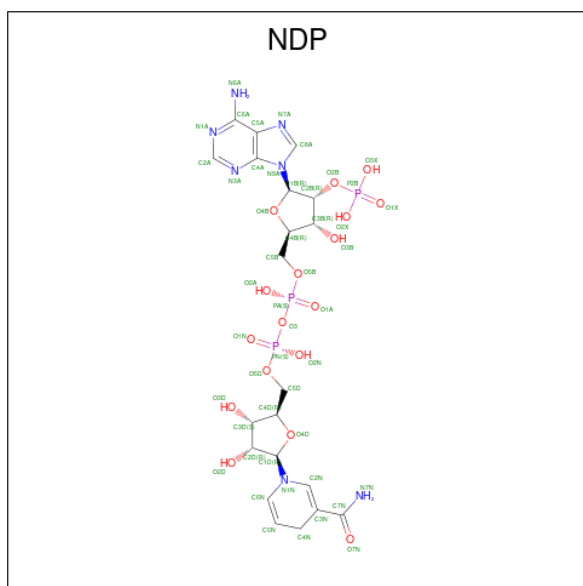
There are 4 unique types of molecules in this entry. The entry contains 1616 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

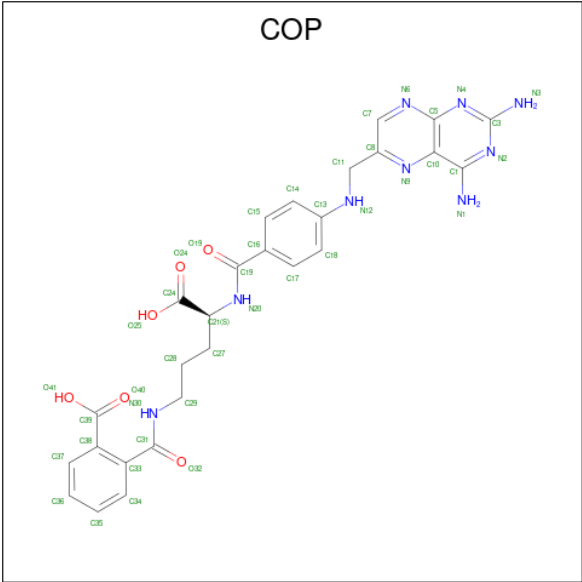
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1502	963	253	279	7	0	0	0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (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-CARBOXY-4-{4-[(2,4-DIAMINO-PTERIDIN-6-YLMETHYL)-AMINO]-BENZOYLAMINO}-BUTYL)-PHTHALAMIC ACID (CCD ID: COP) (formula: $C_{27}H_{27}N_9O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			56	37	10	9		

- Molecule 4 is water.

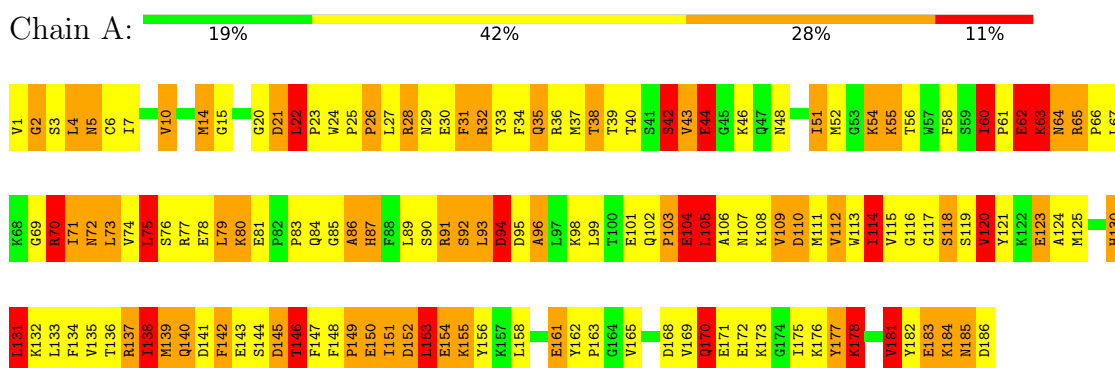
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: DIHYDROFOLATE REDUCTASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.82Å 40.35Å 75.15Å 90.00° 109.74° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	93.4 (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.208 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1616	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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, COP

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	1.09	0/1537	2.95	199/2073 (9.6%)

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	1

There are no bond length outliers.

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	PHE	CA-CB-CG	17.40	131.20	113.80
1	A	62	GLU	CA-C-N	17.02	143.52	120.54
1	A	62	GLU	C-N-CA	17.02	143.52	120.54
1	A	141	ASP	CA-CB-CG	13.44	126.04	112.60
1	A	78	GLU	N-CA-C	11.67	128.67	112.45
1	A	150	GLU	CB-CG-CD	11.61	132.34	112.60
1	A	29	ASN	CA-CB-CG	-10.93	101.67	112.60
1	A	44	GLU	CB-CG-CD	10.54	130.52	112.60
1	A	2	GLY	CA-C-N	10.51	136.53	121.50
1	A	2	GLY	C-N-CA	10.51	136.53	121.50
1	A	79	LEU	CA-C-O	-9.91	110.37	121.87
1	A	25	PRO	CB-CA-C	9.87	120.67	111.39
1	A	87	HIS	CA-CB-CG	9.87	123.67	113.80
1	A	29	ASN	OD1-CG-ND2	9.87	132.47	122.60
1	A	89	LEU	CA-C-O	-9.77	109.89	120.24
1	A	60	ILE	N-CA-CB	9.37	124.32	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ARG	CD-NE-CZ	-9.27	111.42	124.40
1	A	118	SER	N-CA-C	8.99	123.35	112.38
1	A	22	LEU	CB-CA-C	8.87	122.30	109.26
1	A	77	ARG	NE-CZ-NH2	8.76	127.08	119.20
1	A	131	LEU	CA-C-O	-8.72	108.44	120.21
1	A	77	ARG	CD-NE-CZ	-8.67	112.26	124.40
1	A	168	ASP	CA-C-O	8.60	132.78	121.78
1	A	140	GLN	CA-CB-CG	8.37	130.83	114.10
1	A	140	GLN	CB-CG-CD	-8.20	98.65	112.60
1	A	162	TYR	N-CA-CB	-8.13	100.19	110.03
1	A	77	ARG	CA-C-N	8.13	138.95	121.64
1	A	77	ARG	C-N-CA	8.13	138.95	121.64
1	A	6	CYS	CA-C-O	-8.13	111.58	120.36
1	A	77	ARG	NE-CZ-NH1	-8.11	113.39	121.50
1	A	109	VAL	CB-CA-C	-8.10	98.49	110.81
1	A	36	ARG	NE-CZ-NH1	7.91	129.41	121.50
1	A	165	VAL	CB-CA-C	7.91	120.14	110.73
1	A	14	MET	N-CA-CB	-7.89	100.70	112.78
1	A	7	ILE	CB-CA-C	7.85	121.92	110.77
1	A	138	ILE	CB-CA-C	7.74	121.21	111.15
1	A	84	GLN	CA-CB-CG	7.68	129.45	114.10
1	A	136	THR	CA-C-O	-7.61	111.94	120.54
1	A	109	VAL	O-C-N	7.55	130.84	123.14
1	A	62	GLU	CB-CG-CD	7.50	125.36	112.60
1	A	172	GLU	CA-CB-CG	7.47	129.04	114.10
1	A	169	VAL	CA-C-O	7.45	129.53	121.04
1	A	138	ILE	N-CA-C	-7.39	99.13	108.89
1	A	28	ARG	CD-NE-CZ	7.33	134.67	124.40
1	A	132	LYS	N-CA-CB	7.31	122.54	110.85
1	A	184	LYS	CA-C-O	-7.20	111.96	120.60
1	A	30	GLU	N-CA-C	-7.18	102.64	111.40
1	A	89	LEU	O-C-N	7.17	131.66	123.27
1	A	111	MET	CA-C-O	7.14	129.71	121.28
1	A	21	ASP	CA-CB-CG	-7.12	105.48	112.60
1	A	62	GLU	O-C-N	-7.11	113.14	122.59
1	A	63	LYS	CA-C-O	7.09	128.49	120.90
1	A	32	ARG	NH1-CZ-NH2	7.04	128.45	119.30
1	A	142	PHE	CA-CB-CG	-7.02	106.78	113.80
1	A	40	THR	CA-C-O	7.01	128.97	120.62
1	A	135	VAL	N-CA-CB	-7.00	102.66	111.41
1	A	171	GLU	CB-CG-CD	6.98	124.47	112.60
1	A	78	GLU	CB-CA-C	-6.98	96.92	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	LYS	CA-C-O	6.95	126.55	118.90
1	A	152	ASP	CA-CB-CG	-6.94	105.66	112.60
1	A	81	GLU	CA-CB-CG	6.89	127.88	114.10
1	A	95	ASP	N-CA-C	-6.84	102.94	112.45
1	A	154	GLU	CA-CB-CG	6.84	127.77	114.10
1	A	54	LYS	CA-C-O	6.79	127.69	120.70
1	A	110	ASP	CA-C-O	6.77	124.49	119.68
1	A	123	GLU	CA-C-N	6.77	132.99	121.14
1	A	123	GLU	C-N-CA	6.77	132.99	121.14
1	A	168	ASP	CA-CB-CG	6.75	119.35	112.60
1	A	10	VAL	N-CA-C	6.68	118.09	108.48
1	A	32	ARG	CA-C-O	6.61	127.05	119.18
1	A	20	GLY	N-CA-C	-6.59	103.55	114.48
1	A	168	ASP	N-CA-C	6.58	119.82	110.14
1	A	91	ARG	CD-NE-CZ	-6.58	115.19	124.40
1	A	40	THR	CA-C-N	6.57	133.31	122.07
1	A	40	THR	C-N-CA	6.57	133.31	122.07
1	A	3	SER	N-CA-CB	-6.56	99.78	109.95
1	A	91	ARG	CA-CB-CG	-6.55	100.99	114.10
1	A	135	VAL	N-CA-C	6.55	117.27	107.51
1	A	104	GLU	CA-C-O	6.53	126.95	119.18
1	A	3	SER	N-CA-C	6.46	120.04	109.76
1	A	120	VAL	N-CA-CB	6.45	119.31	110.54
1	A	172	GLU	CA-C-O	-6.45	112.35	120.28
1	A	137	ARG	NE-CZ-NH1	6.38	127.88	121.50
1	A	137	ARG	NH1-CZ-NH2	-6.37	111.02	119.30
1	A	56	THR	N-CA-CB	6.37	119.24	110.01
1	A	119	SER	N-CA-C	-6.37	106.05	113.88
1	A	170	GLN	OE1-CD-NE2	6.34	128.94	122.60
1	A	142	PHE	O-C-N	6.31	131.00	123.24
1	A	145	ASP	CA-C-N	6.31	131.83	121.86
1	A	145	ASP	C-N-CA	6.31	131.83	121.86
1	A	74	VAL	CB-CA-C	6.28	119.50	110.33
1	A	60	ILE	CB-CG1-CD1	6.27	126.96	113.80
1	A	86	ALA	CA-C-O	-6.25	115.00	121.87
1	A	63	LYS	CA-C-N	6.22	133.63	122.38
1	A	63	LYS	C-N-CA	6.22	133.63	122.38
1	A	114	ILE	N-CA-CB	6.20	118.73	111.66
1	A	123	GLU	CB-CG-CD	-6.17	102.12	112.60
1	A	183	GLU	CB-CG-CD	-6.12	102.19	112.60
1	A	169	VAL	CB-CA-C	6.12	120.45	111.33
1	A	31	PHE	N-CA-CB	6.08	119.59	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	PHE	CA-C-N	6.02	128.27	120.44
1	A	34	PHE	C-N-CA	6.02	128.27	120.44
1	A	35	GLN	N-CA-C	5.98	117.47	111.07
1	A	36	ARG	CD-NE-CZ	5.95	132.72	124.40
1	A	94	ASP	CA-CB-CG	-5.93	106.67	112.60
1	A	172	GLU	N-CA-C	-5.92	98.20	108.69
1	A	163	PRO	CB-CA-C	-5.91	104.03	111.71
1	A	140	GLN	N-CA-CB	5.90	121.49	111.57
1	A	149	PRO	CB-CA-C	5.90	119.13	111.64
1	A	51	ILE	CA-CB-CG2	5.89	120.51	110.50
1	A	32	ARG	NE-CZ-NH2	-5.87	113.92	119.20
1	A	72	ASN	CA-CB-CG	-5.85	106.75	112.60
1	A	31	PHE	CA-C-O	-5.85	113.49	120.10
1	A	75	LEU	CA-C-N	5.84	132.50	121.69
1	A	75	LEU	C-N-CA	5.84	132.50	121.69
1	A	93	LEU	CA-C-N	5.84	129.95	120.60
1	A	93	LEU	C-N-CA	5.84	129.95	120.60
1	A	65	ARG	N-CA-C	5.83	119.12	110.32
1	A	62	GLU	CA-C-O	5.77	128.77	120.51
1	A	123	GLU	CG-CD-OE1	-5.72	105.25	118.40
1	A	147	PHE	N-CA-C	5.71	118.53	109.50
1	A	120	VAL	N-CA-C	-5.71	104.79	110.62
1	A	141	ASP	CB-CG-OD1	5.70	131.51	118.40
1	A	153	LEU	CA-C-O	-5.70	112.36	120.51
1	A	22	LEU	N-CA-C	-5.67	102.89	109.93
1	A	120	VAL	CB-CA-C	-5.67	104.48	112.14
1	A	143	GLU	CA-C-N	5.67	131.47	122.62
1	A	143	GLU	C-N-CA	5.67	131.47	122.62
1	A	149	PRO	CA-C-N	5.66	128.88	120.90
1	A	149	PRO	C-N-CA	5.66	128.88	120.90
1	A	130	HIS	CA-CB-CG	5.66	119.46	113.80
1	A	4	LEU	CA-C-N	5.64	131.67	122.81
1	A	4	LEU	C-N-CA	5.64	131.67	122.81
1	A	136	THR	N-CA-C	-5.63	100.11	109.46
1	A	117	GLY	CA-C-N	5.61	129.57	120.60
1	A	117	GLY	C-N-CA	5.61	129.57	120.60
1	A	78	GLU	CA-CB-CG	5.60	125.30	114.10
1	A	74	VAL	N-CA-CB	-5.58	103.38	111.52
1	A	92	SER	CA-C-O	-5.55	115.34	121.33
1	A	38	THR	CA-C-N	5.52	130.02	120.58
1	A	38	THR	C-N-CA	5.52	130.02	120.58
1	A	141	ASP	O-C-N	5.52	130.22	123.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	GLU	CB-CG-CD	5.51	121.97	112.60
1	A	71	ILE	CB-CG1-CD1	5.51	125.37	113.80
1	A	78	GLU	CB-CG-CD	-5.48	103.28	112.60
1	A	15	GLY	CA-C-N	5.48	128.37	121.85
1	A	15	GLY	C-N-CA	5.48	128.37	121.85
1	A	105	LEU	N-CA-C	-5.47	105.25	113.89
1	A	155	LYS	N-CA-C	-5.47	107.26	114.04
1	A	25	PRO	N-CA-C	-5.46	105.22	110.47
1	A	154	GLU	CA-C-O	5.46	125.92	119.48
1	A	60	ILE	CA-CB-CG1	5.45	119.66	110.40
1	A	151	ILE	CB-CA-C	5.44	117.66	110.91
1	A	178	LYS	CA-CB-CG	5.43	124.95	114.10
1	A	44	GLU	CB-CA-C	-5.42	101.45	109.90
1	A	84	GLN	CB-CA-C	5.42	118.90	110.67
1	A	3	SER	CA-C-O	-5.40	114.53	120.69
1	A	73	LEU	CB-CA-C	5.35	119.50	109.71
1	A	30	GLU	CA-C-O	5.35	126.27	120.55
1	A	65	ARG	NH1-CZ-NH2	5.35	126.25	119.30
1	A	131	LEU	O-C-N	5.34	130.01	123.44
1	A	137	ARG	CA-CB-CG	5.34	124.78	114.10
1	A	96	ALA	N-CA-C	-5.32	105.38	111.07
1	A	153	LEU	CA-C-N	-5.29	114.22	122.37
1	A	153	LEU	C-N-CA	-5.29	114.22	122.37
1	A	67	LEU	CB-CA-C	5.29	119.35	110.88
1	A	111	MET	CA-C-N	-5.27	116.65	123.19
1	A	111	MET	C-N-CA	-5.27	116.65	123.19
1	A	181	VAL	CA-CB-CG2	5.24	119.30	110.40
1	A	147	PHE	CA-CB-CG	5.18	118.98	113.80
1	A	136	THR	N-CA-CB	5.18	118.70	110.16
1	A	71	ILE	N-CA-CB	5.18	116.90	111.00
1	A	56	THR	CA-C-N	5.17	127.47	120.65
1	A	56	THR	C-N-CA	5.17	127.47	120.65
1	A	145	ASP	CB-CG-OD1	5.16	130.28	118.40
1	A	28	ARG	NH1-CZ-NH2	-5.16	112.60	119.30
1	A	139	MET	CB-CA-C	5.15	119.69	112.07
1	A	64	ASN	N-CA-C	5.14	119.53	113.16
1	A	177	TYR	CA-C-O	-5.14	115.24	120.89
1	A	60	ILE	CB-CA-C	-5.11	102.07	111.36
1	A	63	LYS	CB-CA-C	-5.10	102.65	110.81
1	A	101	GLU	CA-CB-CG	5.10	124.29	114.10
1	A	67	LEU	N-CA-CB	-5.09	101.84	109.88
1	A	36	ARG	CA-C-O	-5.08	115.46	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	VAL	CA-C-O	-5.06	114.95	120.72
1	A	81	GLU	O-C-N	5.05	127.75	121.79
1	A	101	GLU	CB-CA-C	-5.05	100.08	110.38
1	A	147	PHE	N-CA-CB	-5.05	102.19	111.37
1	A	168	ASP	CA-C-N	5.04	127.83	120.98
1	A	168	ASP	C-N-CA	5.04	127.83	120.98
1	A	64	ASN	CA-C-O	-5.02	113.20	119.28
1	A	140	GLN	O-C-N	5.02	128.31	123.29
1	A	26	PRO	CA-C-O	-5.02	115.85	121.32
1	A	58	PHE	CA-C-O	-5.01	110.89	118.91
1	A	131	LEU	CB-CA-C	5.01	118.32	109.80
1	A	144	SER	N-CA-C	5.01	117.42	109.50
1	A	146	THR	CB-CA-C	5.01	117.55	110.24
1	A	161	GLU	CB-CA-C	-5.00	100.46	110.42
1	A	134	PHE	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	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	121	0
2	A	48	0	26	7	0
3	A	56	0	20	2	0
4	A	10	0	0	1	0
All	All	1616	0	1557	126	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 40.

All (126) 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:79:LEU:O	1:A:91:ARG:NH2	1.81	1.12
2:A:187:NDP:H52A	2:A:187:NDP:H8A	1.50	0.94
1:A:1:VAL:HG13	1:A:2:GLY:H	1.30	0.93
1:A:4:LEU:HD12	1:A:112:VAL:CG2	1.99	0.92
1:A:62:GLU:OE2	1:A:65:ARG:NH2	2.03	0.92
1:A:54:LYS:HD3	2:A:187:NDP:O2X	1.73	0.88
1:A:35:GLN:O	1:A:39:THR:OG1	1.94	0.85
1:A:72:ASN:H	1:A:87:HIS:HD2	1.29	0.81
1:A:72:ASN:H	1:A:87:HIS:CD2	2.03	0.74
1:A:114:ILE:HD13	1:A:124:ALA:HB1	1.71	0.71
1:A:161:GLU:O	1:A:161:GLU:HG2	1.88	0.71
1:A:91:ARG:HG2	1:A:91:ARG:NH1	2.07	0.69
1:A:145:ASP:OD1	1:A:146:THR:HG22	1.92	0.69
1:A:130:HIS:HB2	1:A:185:ASN:CG	2.19	0.68
1:A:96:ALA:O	1:A:99:LEU:HB3	1.93	0.68
1:A:151:ILE:HA	4:A:193:HOH:O	1.92	0.68
1:A:28:ARG:O	1:A:32:ARG:HG3	1.94	0.68
1:A:42:SER:OG	1:A:110:ASP:OD2	2.13	0.66
1:A:114:ILE:HD13	1:A:124:ALA:CB	2.26	0.65
1:A:76:SER:O	1:A:91:ARG:NH1	2.30	0.65
1:A:72:ASN:N	1:A:72:ASN:HD22	1.94	0.64
1:A:52:MET:HA	1:A:116:GLY:O	1.97	0.64
1:A:109:VAL:HG13	1:A:109:VAL:O	1.99	0.63
1:A:60:ILE:HG21	1:A:64:ASN:HB3	1.81	0.63
1:A:54:LYS:NZ	2:A:187:NDP:O2X	2.30	0.62
1:A:130:HIS:HB2	1:A:185:ASN:ND2	2.14	0.62
1:A:93:LEU:HD22	1:A:123:GLU:HG3	1.82	0.62
1:A:66:PRO:HG3	1:A:85:GLY:O	1.99	0.62
1:A:21:ASP:OD1	1:A:22:LEU:N	2.28	0.62
1:A:46:LYS:HE2	1:A:107:ASN:O	2.01	0.60
1:A:4:LEU:HD12	1:A:112:VAL:HG21	1.83	0.60
1:A:91:ARG:HG2	1:A:91:ARG:HH11	1.66	0.60
1:A:120:VAL:O	1:A:124:ALA:HB2	2.04	0.58
1:A:60:ILE:HG22	1:A:61:PRO:HD2	1.86	0.57
1:A:161:GLU:O	1:A:161:GLU:CG	2.51	0.57
3:A:188[A]:COP:O40	3:A:188[A]:COP:O32	2.22	0.57
1:A:69:GLY:C	1:A:70:ARG:HG3	2.29	0.57
1:A:109:VAL:O	1:A:109:VAL:CG1	2.53	0.56
1:A:44:GLU:O	1:A:44:GLU:HG3	2.05	0.56
1:A:61:PRO:O	1:A:63:LYS:N	2.38	0.56
1:A:99:LEU:HG	1:A:105:LEU:HD23	1.86	0.56
1:A:60:ILE:HG22	1:A:64:ASN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:SER:HB3	2:A:187:NDP:O1N	2.06	0.55
1:A:133:LEU:O	1:A:181:VAL:HA	2.06	0.55
1:A:10:VAL:CG2	1:A:14:MET:HA	2.36	0.55
1:A:4:LEU:CD1	1:A:112:VAL:CG2	2.81	0.55
1:A:170:GLN:O	1:A:176:LYS:HA	2.08	0.54
1:A:121:TYR:O	1:A:124:ALA:HB3	2.08	0.53
1:A:60:ILE:CG2	1:A:64:ASN:HB3	2.39	0.53
1:A:131:LEU:HD23	1:A:184:LYS:HE2	1.91	0.53
1:A:4:LEU:CD1	1:A:112:VAL:HG21	2.40	0.52
1:A:55:LYS:HB2	1:A:55:LYS:HZ3	1.74	0.52
1:A:94:ASP:O	1:A:98:LYS:HE3	2.08	0.52
1:A:1:VAL:CG1	1:A:2:GLY:H	2.09	0.52
1:A:152:ASP:HB3	1:A:155:LYS:HB3	1.91	0.52
1:A:93:LEU:HD13	1:A:120:VAL:HG12	1.91	0.52
1:A:51:ILE:HG12	1:A:73:LEU:HD22	1.91	0.51
1:A:93:LEU:O	1:A:96:ALA:HB3	2.11	0.51
2:A:187:NDP:H6N	2:A:187:NDP:H52N	1.93	0.51
1:A:105:LEU:O	1:A:109:VAL:HG12	2.11	0.50
1:A:42:SER:HG	1:A:110:ASP:CG	2.19	0.50
1:A:103:PRO:HA	1:A:106:ALA:HB3	1.93	0.50
1:A:71:ILE:C	1:A:72:ASN:HD22	2.20	0.49
1:A:152:ASP:O	1:A:154:GLU:N	2.46	0.49
1:A:83:PRO:HG2	1:A:86:ALA:HB2	1.95	0.49
1:A:33:TYR:O	1:A:37:MET:HG2	2.13	0.48
1:A:1:VAL:HG13	1:A:2:GLY:N	2.12	0.48
1:A:4:LEU:HA	1:A:112:VAL:HG22	1.94	0.48
1:A:10:VAL:HG22	1:A:14:MET:HA	1.96	0.48
1:A:75:LEU:HA	1:A:90:SER:O	2.14	0.47
1:A:72:ASN:N	1:A:87:HIS:HD2	2.06	0.47
1:A:148:PHE:CD1	1:A:149:PRO:HD2	2.49	0.47
1:A:170:GLN:HE21	1:A:170:GLN:HA	1.80	0.47
1:A:155:LYS:HE3	1:A:184:LYS:HD2	1.97	0.47
1:A:177:TYR:C	1:A:177:TYR:CD1	2.92	0.47
1:A:38:THR:O	1:A:48:ASN:ND2	2.33	0.46
1:A:153:LEU:HD23	1:A:153:LEU:H	1.81	0.46
1:A:138:ILE:HG23	1:A:175:ILE:CG2	2.45	0.46
1:A:60:ILE:HG22	1:A:64:ASN:CB	2.45	0.46
1:A:24:TRP:HB3	1:A:142:PHE:CZ	2.51	0.46
1:A:108:LYS:NZ	1:A:108:LYS:HB2	2.31	0.46
1:A:114:ILE:O	1:A:114:ILE:HG22	2.16	0.46
1:A:152:ASP:C	1:A:154:GLU:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ASN:ND2	1:A:5:ASN:N	2.63	0.45
1:A:62:GLU:H	1:A:62:GLU:CD	2.25	0.45
1:A:152:ASP:C	1:A:154:GLU:N	2.74	0.45
1:A:102:GLN:O	1:A:104:GLU:N	2.50	0.45
1:A:186:ASP:OD1	1:A:186:ASP:C	2.60	0.45
1:A:177:TYR:CD1	1:A:177:TYR:O	2.69	0.45
1:A:4:LEU:HD12	1:A:112:VAL:HG22	1.91	0.45
1:A:60:ILE:CG2	1:A:64:ASN:CB	2.94	0.45
1:A:51:ILE:HD13	1:A:51:ILE:HG21	1.57	0.44
1:A:26:PRO:O	1:A:173:LYS:CE	2.65	0.44
2:A:187:NDP:H8A	2:A:187:NDP:C5B	2.33	0.44
1:A:60:ILE:HG22	1:A:61:PRO:CD	2.48	0.44
1:A:103:PRO:HA	1:A:106:ALA:CB	2.48	0.44
1:A:104:GLU:H	1:A:104:GLU:HG2	1.29	0.44
1:A:158:LEU:HB2	1:A:182:TYR:CE2	2.53	0.43
1:A:23:PRO:HB2	1:A:142:PHE:HB3	2.00	0.43
1:A:21:ASP:CG	1:A:22:LEU:H	2.19	0.43
1:A:61:PRO:C	1:A:63:LYS:N	2.77	0.43
1:A:94:ASP:O	1:A:98:LYS:HB2	2.18	0.43
1:A:170:GLN:HE21	1:A:170:GLN:CA	2.31	0.43
1:A:55:LYS:HB2	1:A:55:LYS:NZ	2.33	0.42
1:A:131:LEU:CD2	1:A:156:TYR:OH	2.67	0.42
1:A:138:ILE:CG2	1:A:142:PHE:HE1	2.32	0.42
1:A:151:ILE:HD13	1:A:151:ILE:HG21	1.77	0.42
1:A:175:ILE:HG21	1:A:175:ILE:HD13	1.67	0.42
1:A:5:ASN:O	1:A:113:TRP:HA	2.19	0.42
1:A:98:LYS:HE3	1:A:98:LYS:HB2	1.65	0.42
1:A:124:ALA:O	1:A:131:LEU:HD22	2.19	0.42
1:A:137:ARG:HG3	1:A:178:LYS:NZ	2.35	0.41
1:A:60:ILE:O	1:A:65:ARG:NH2	2.44	0.41
1:A:43:VAL:HG11	1:A:46:LYS:HD2	2.03	0.41
1:A:54:LYS:CD	2:A:187:NDP:O2X	2.58	0.41
1:A:61:PRO:C	1:A:63:LYS:H	2.27	0.41
1:A:102:GLN:H	1:A:102:GLN:HG2	1.62	0.41
1:A:125:MET:HA	1:A:131:LEU:HD21	2.02	0.41
1:A:120:VAL:O	1:A:124:ALA:CB	2.67	0.40
1:A:183:GLU:CG	1:A:184:LYS:N	2.84	0.40
1:A:139:MET:HE2	1:A:139:MET:HB3	1.96	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%)	168 (91%)	12 (6%)	4 (2%)	5 9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	153	LEU
1	A	42	SER
1	A	103	PRO

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%)	137 (82%)	31 (18%)	1 3

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	22	LEU
1	A	27	LEU
1	A	42	SER
1	A	43	VAL
1	A	44	GLU
1	A	55	LYS

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Mol	Chain	Res	Type
1	A	60	ILE
1	A	62	GLU
1	A	63	LYS
1	A	70	ARG
1	A	75	LEU
1	A	80	LYS
1	A	92	SER
1	A	94	ASP
1	A	104	GLU
1	A	105	LEU
1	A	112	VAL
1	A	114	ILE
1	A	115	VAL
1	A	120	VAL
1	A	131	LEU
1	A	138	ILE
1	A	140	GLN
1	A	146	THR
1	A	150	GLU
1	A	153	LEU
1	A	170	GLN
1	A	178	LYS
1	A	181	VAL
1	A	185	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	12	GLN
1	A	87	HIS
1	A	102	GLN
1	A	126	ASN
1	A	170	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	COP	A	188[A]	-	45,45,45	1.55	7 (15%)	60,62,62	3.49	21 (35%)
3	COP	A	188[B]	-	45,45,45	1.57	6 (13%)	60,62,62	3.31	22 (36%)
2	NDP	A	187	-	51,52,52	2.70	17 (33%)	71,80,80	2.48	28 (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	COP	A	188[A]	-	-	5/32/32/32	0/4/4/4
3	COP	A	188[B]	-	-	9/32/32/32	0/4/4/4
2	NDP	A	187	-	-	9/34/77/77	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	O4B-C4B	-9.44	1.24	1.45
2	A	187	NDP	P2B-O2B	6.69	1.71	1.59
2	A	187	NDP	C5A-C6A	5.87	1.57	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	C5A-C4A	-4.80	1.30	1.39
2	A	187	NDP	C6A-N1A	-4.59	1.22	1.35
3	A	188[B]	COP	O40-C39	4.59	1.36	1.22
3	A	188[A]	COP	C5-N6	-4.52	1.30	1.37
3	A	188[B]	COP	C5-N6	-4.52	1.30	1.37
3	A	188[A]	COP	O40-C39	4.17	1.34	1.22
2	A	187	NDP	C3B-C4B	4.12	1.63	1.53
2	A	187	NDP	C4A-N9A	-3.90	1.29	1.37
2	A	187	NDP	O3B-C3B	3.69	1.52	1.43
2	A	187	NDP	C4N-C3N	3.46	1.56	1.50
3	A	188[B]	COP	C31-N30	3.32	1.41	1.33
2	A	187	NDP	C1D-N1N	3.26	1.55	1.46
2	A	187	NDP	PN-O1N	-3.26	1.39	1.50
3	A	188[A]	COP	C31-N30	3.08	1.40	1.33
2	A	187	NDP	C5A-N7A	2.98	1.44	1.39
3	A	188[A]	COP	O25-C24	-2.73	1.22	1.30
3	A	188[B]	COP	O25-C24	-2.73	1.22	1.30
3	A	188[A]	COP	C29-N30	2.70	1.52	1.46
3	A	188[B]	COP	C29-N30	2.68	1.52	1.46
3	A	188[A]	COP	O41-C39	-2.64	1.22	1.30
2	A	187	NDP	PA-O5B	2.50	1.69	1.59
2	A	187	NDP	P2B-O2X	-2.40	1.45	1.54
3	A	188[A]	COP	C3-N2	-2.40	1.31	1.35
3	A	188[B]	COP	C3-N2	-2.40	1.31	1.35
2	A	187	NDP	O2B-C2B	-2.23	1.36	1.44
2	A	187	NDP	PA-O2A	-2.15	1.45	1.55
2	A	187	NDP	C8A-N9A	-2.06	1.34	1.37

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188[A]	COP	C29-N30-C31	19.40	165.99	122.11
3	A	188[B]	COP	C29-N30-C31	15.52	157.21	122.11
2	A	187	NDP	P2B-O2B-C2B	6.84	141.70	123.43
3	A	188[B]	COP	C28-C29-N30	6.54	130.55	112.20
2	A	187	NDP	N6A-C6A-N1A	6.14	132.06	118.38
2	A	187	NDP	O3B-C3B-C4B	-6.05	93.70	111.08
3	A	188[A]	COP	O25-C24-O24	5.63	136.84	124.08
3	A	188[B]	COP	O25-C24-O24	5.63	136.84	124.08
2	A	187	NDP	C5A-C6A-N6A	-5.46	109.77	123.29
3	A	188[A]	COP	C27-C21-C24	-5.37	97.60	110.35
3	A	188[B]	COP	C27-C21-C24	-5.37	97.60	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188[A]	COP	C24-C21-N20	5.25	122.76	110.57
3	A	188[B]	COP	C24-C21-N20	5.25	122.76	110.57
3	A	188[A]	COP	C28-C29-N30	4.86	125.82	112.20
2	A	187	NDP	C4A-N9A-C8A	4.78	110.75	105.74
3	A	188[A]	COP	C3-N4-C5	4.54	120.38	115.48
3	A	188[B]	COP	C3-N4-C5	4.54	120.38	115.48
3	A	188[B]	COP	O41-C39-O40	4.53	133.10	123.35
3	A	188[A]	COP	C21-N20-C19	4.47	132.30	121.56
3	A	188[B]	COP	C21-N20-C19	4.47	132.30	121.56
3	A	188[B]	COP	C33-C31-N30	4.29	125.65	117.32
3	A	188[A]	COP	C7-C8-N9	4.26	123.64	120.87
3	A	188[B]	COP	C7-C8-N9	4.26	123.64	120.87
2	A	187	NDP	C4B-O4B-C1B	4.25	118.84	109.47
3	A	188[B]	COP	O32-C31-C33	-4.22	113.31	121.03
3	A	188[A]	COP	O19-C19-C16	-4.11	112.75	120.90
3	A	188[B]	COP	O19-C19-C16	-4.11	112.75	120.90
3	A	188[A]	COP	N6-C5-N4	4.10	120.23	115.77
3	A	188[B]	COP	N6-C5-N4	4.10	120.23	115.77
2	A	187	NDP	O2B-P2B-O1X	-3.88	95.49	109.33
3	A	188[A]	COP	N4-C3-N2	-3.88	122.28	127.21
3	A	188[B]	COP	N4-C3-N2	-3.88	122.28	127.21
2	A	187	NDP	O3-PN-O1N	3.85	122.30	110.70
2	A	187	NDP	O3X-P2B-O2X	3.84	122.18	107.80
2	A	187	NDP	C5B-C4B-C3B	-3.82	101.47	115.21
3	A	188[A]	COP	C8-C7-N6	-3.80	119.50	123.14
3	A	188[B]	COP	C8-C7-N6	-3.80	119.50	123.14
3	A	188[A]	COP	C16-C19-N20	3.78	124.05	117.04
3	A	188[B]	COP	C16-C19-N20	3.78	124.05	117.04
2	A	187	NDP	O4B-C1B-C2B	-3.76	100.12	106.59
3	A	188[A]	COP	C1-C10-N9	3.69	123.17	120.33
3	A	188[B]	COP	C1-C10-N9	3.69	123.17	120.33
3	A	188[A]	COP	O32-C31-C33	-3.67	114.31	121.03
2	A	187	NDP	C6N-N1N-C2N	3.66	123.23	119.32
2	A	187	NDP	O2B-C2B-C1B	-3.54	97.62	110.05
3	A	188[A]	COP	C27-C28-C29	-3.53	101.88	112.07
2	A	187	NDP	O5B-PA-O1A	-3.45	95.26	108.94
2	A	187	NDP	O2A-PA-O1A	3.11	126.92	112.44
2	A	187	NDP	C3N-C7N-N7N	3.06	123.10	117.67
3	A	188[A]	COP	O24-C24-C21	-2.99	112.63	122.26
3	A	188[B]	COP	O24-C24-C21	-2.99	112.63	122.26
3	A	188[A]	COP	O41-C39-C38	2.94	123.63	115.28
2	A	187	NDP	O5B-C5B-C4B	-2.93	99.01	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188[B]	COP	C27-C28-C29	-2.85	103.85	112.07
3	A	188[A]	COP	O41-C39-O40	-2.81	117.31	123.35
3	A	188[B]	COP	O41-C39-C38	-2.65	107.75	115.28
2	A	187	NDP	C5A-N7A-C8A	-2.62	99.33	103.45
3	A	188[B]	COP	C37-C38-C33	2.62	122.20	119.26
2	A	187	NDP	PN-O5D-C5D	2.55	135.94	121.35
2	A	187	NDP	C2B-C3B-C4B	-2.51	96.59	101.99
3	A	188[A]	COP	C27-C21-N20	-2.50	105.96	110.91
3	A	188[B]	COP	C27-C21-N20	-2.50	105.96	110.91
2	A	187	NDP	O4D-C4D-C3D	-2.47	100.24	105.15
2	A	187	NDP	C1D-N1N-C2N	-2.47	117.07	121.14
2	A	187	NDP	O2A-PA-O3	2.41	113.79	107.27
2	A	187	NDP	C1B-N9A-C8A	-2.37	121.83	127.09
2	A	187	NDP	O4B-C1B-N9A	2.14	112.19	108.09
3	A	188[A]	COP	C33-C31-N30	2.12	121.45	117.32
2	A	187	NDP	C2D-C3D-C4D	-2.05	98.65	102.61
2	A	187	NDP	C4A-C5A-N7A	2.05	112.92	110.58
2	A	187	NDP	O2N-PN-O3	-2.00	101.86	107.27

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	187	NDP	O4D-C4D-C5D-O5D
2	A	187	NDP	C3D-C4D-C5D-O5D
3	A	188[A]	COP	C33-C31-N30-C29
3	A	188[B]	COP	C33-C31-N30-C29
3	A	188[A]	COP	O32-C31-N30-C29
3	A	188[B]	COP	O32-C31-N30-C29
3	A	188[A]	COP	C28-C29-N30-C31
3	A	188[B]	COP	C28-C29-N30-C31
3	A	188[A]	COP	N20-C21-C27-C28
3	A	188[B]	COP	N20-C21-C27-C28
3	A	188[B]	COP	N30-C31-C33-C38
3	A	188[A]	COP	C27-C28-C29-N30
3	A	188[B]	COP	O32-C31-C33-C38
2	A	187	NDP	C5D-O5D-PN-O1N
3	A	188[B]	COP	C27-C28-C29-N30
3	A	188[B]	COP	C37-C38-C39-O41
3	A	188[B]	COP	C37-C38-C39-O40
2	A	187	NDP	O4D-C1D-N1N-C2N
2	A	187	NDP	C2N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
2	A	187	NDP	C2D-C1D-N1N-C2N
2	A	187	NDP	C1B-C2B-O2B-P2B
2	A	187	NDP	PN-O3-PA-O1A
2	A	187	NDP	PA-O3-PN-O2N

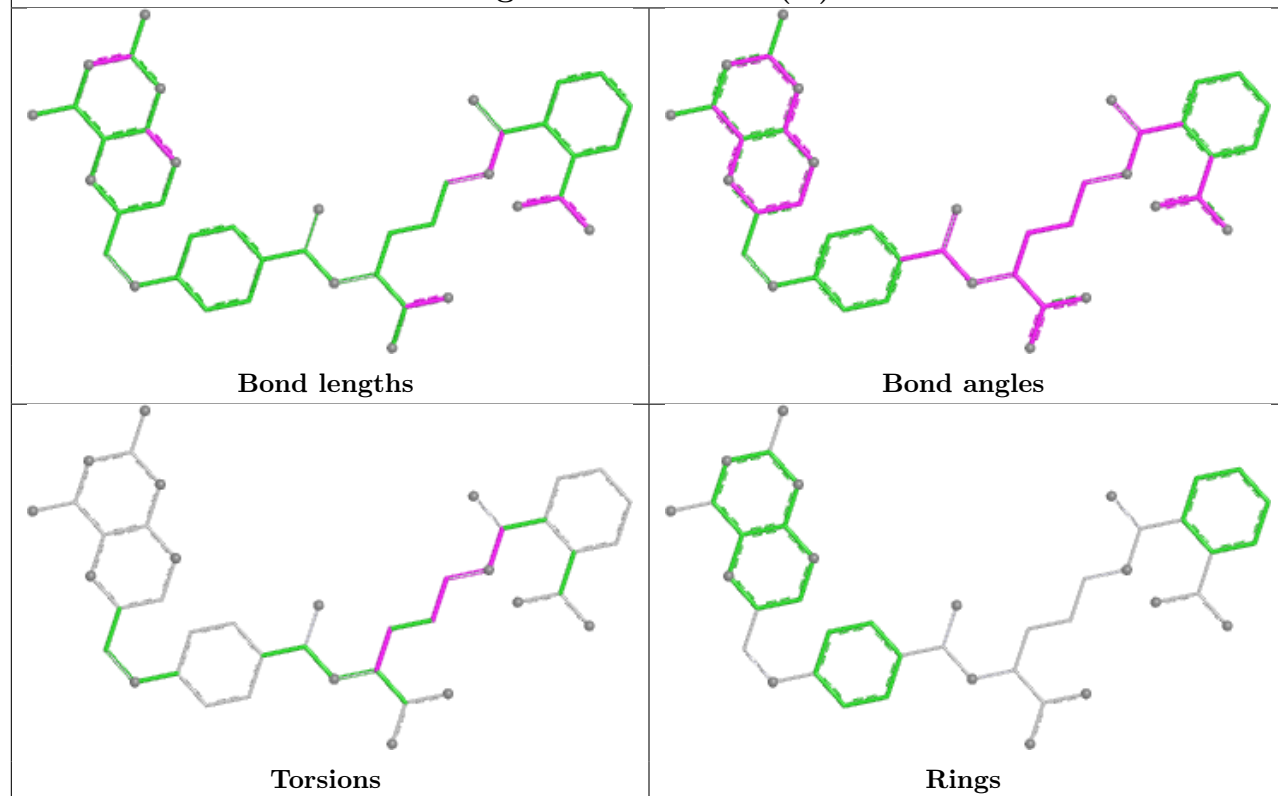
There are no ring outliers.

2 monomers are involved in 9 short contacts:

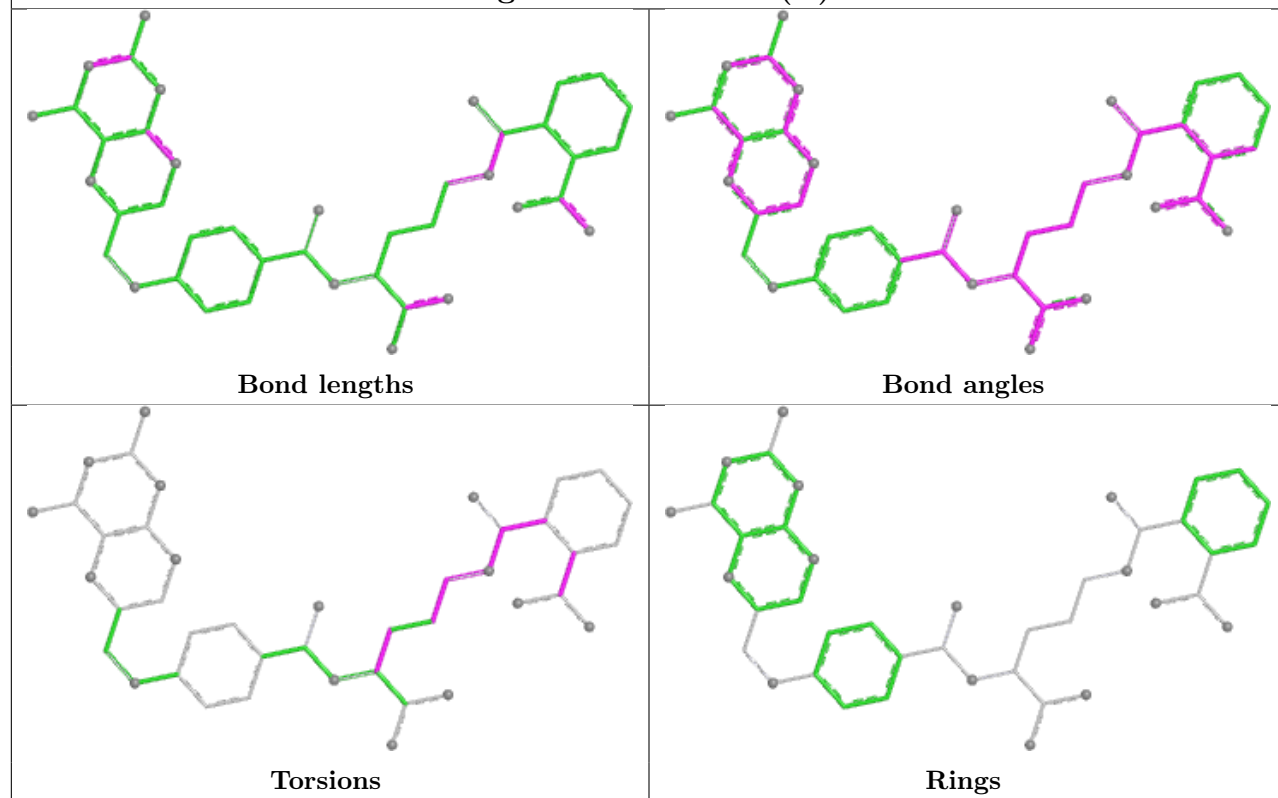
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	188[A]	COP	2	0
2	A	187	NDP	7	0

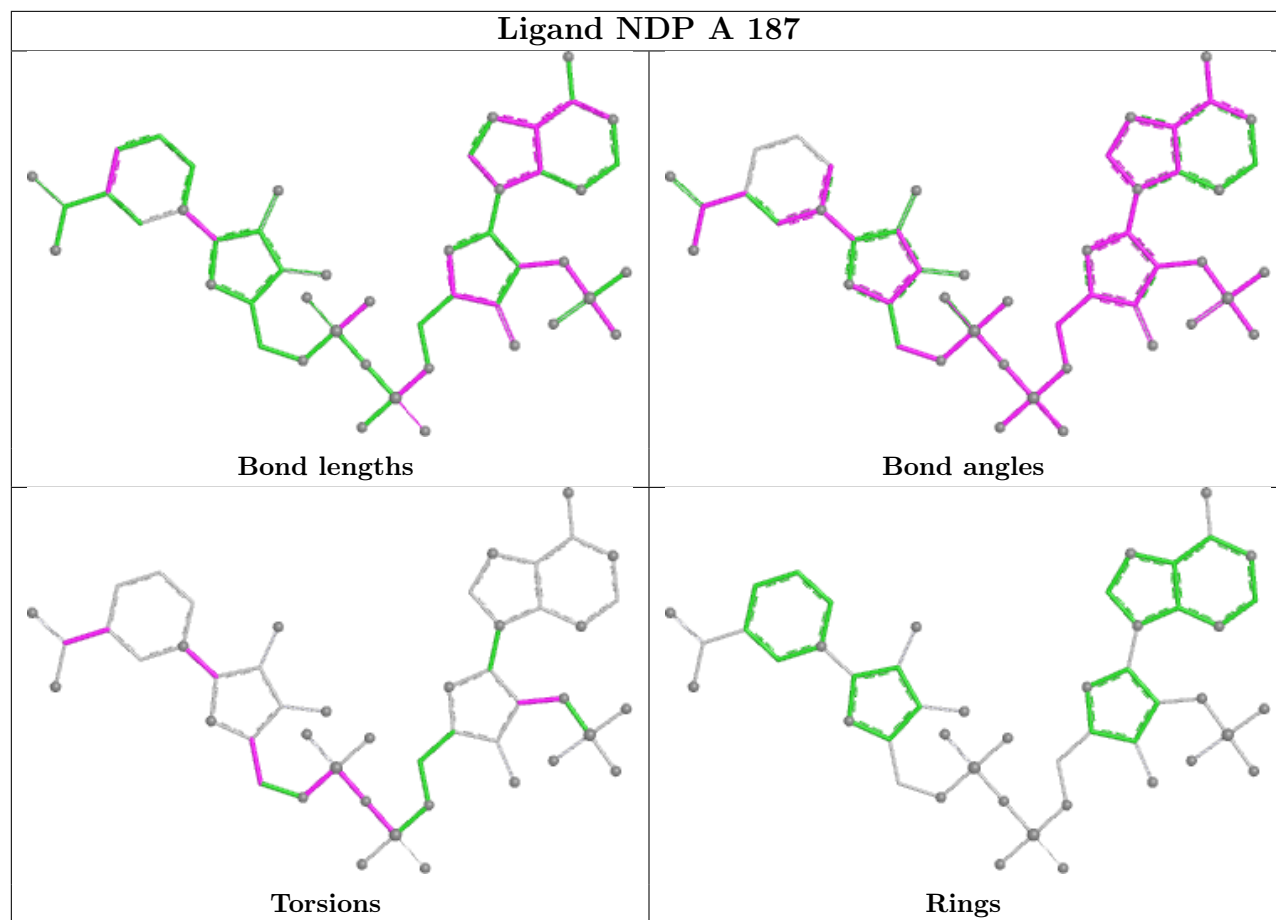
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand COP A 188 (A)



Ligand COP A 188 (B)





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.