Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 01:59 PM EDT

PDB ID	:	1HFQ
Title	:	COMPARISON OF TERNARY CRYSTAL COMPLEXES OF HUMAN DIHYDROFOLATE REDUCTASE WITH NADPH AND A CLASSICAL ANTITUMOR FUROPYRIMDINE
Authors	:	Cody, V.; Galitsky, N.; Luft, J.R.; Pangborn, W.; Blakley, R.L.; Gangjee, A.
Deposited on	:	1997-11-04
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

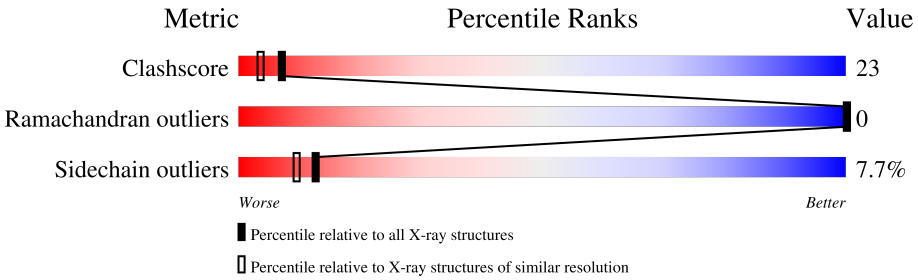
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	186	31% 44% 23% .

2 Entry composition

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.

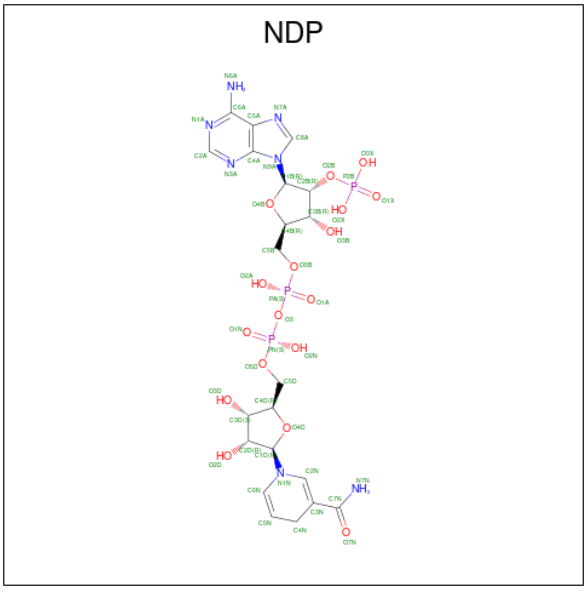
- Molecule 1 is a protein called DIHYDROFOLATE REDUCTASE.

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

There is a discrepancy between the modelled and reference sequences:

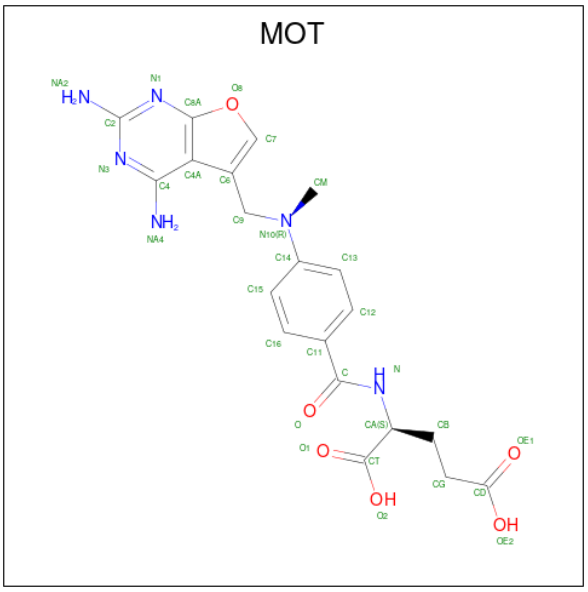
Chain	Residue	Modelled	Actual	Comment	Reference
A	31	SER	PHE	engineered mutation	UNP P00374

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: 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 (three-letter code: MOT) (formula: $C_{20}H_{22}N_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 32 20 6 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	51	Total O 51 51	0	0

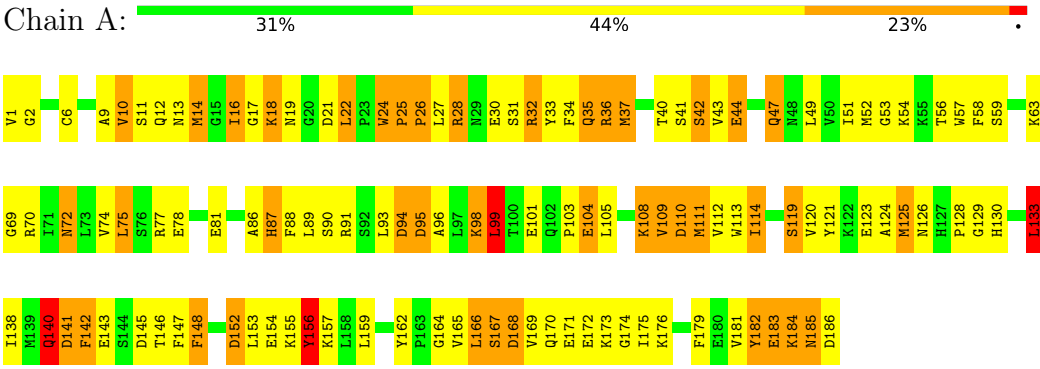
3 Residue-property plots (i)

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

Note EDS was not executed.

• Molecule 1: DIHYDROFOLATE REDUCTASE

Chain A:



4 Data and refinement statistics (i)

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: 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	2.04	38/1531 (2.5%)	3.22	208/2065 (10.1%)

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 (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	SER	CB-OG	15.09	1.61	1.42
1	A	9	ALA	C-O	8.47	1.39	1.23
1	A	183	GLU	CD-OE2	-8.04	1.16	1.25
1	A	31	SER	CA-CB	7.77	1.64	1.52
1	A	172	GLU	CD-OE2	7.60	1.34	1.25
1	A	91	ARG	CZ-NH1	7.49	1.42	1.33
1	A	34	PHE	N-CA	6.91	1.60	1.46
1	A	91	ARG	CZ-NH2	6.85	1.42	1.33
1	A	121	TYR	CD1-CE1	6.85	1.49	1.39
1	A	134	PHE	CG-CD2	6.70	1.48	1.38
1	A	136	THR	C-O	6.18	1.35	1.23
1	A	16	ILE	CB-CG1	6.18	1.71	1.54
1	A	59	SER	CB-OG	-6.08	1.34	1.42
1	A	185	ASN	CG-OD1	6.05	1.37	1.24
1	A	162	TYR	CE1-CZ	5.93	1.46	1.38
1	A	36	ARG	CZ-NH2	5.91	1.40	1.33
1	A	34	PHE	CB-CG	5.87	1.61	1.51
1	A	121	TYR	CE1-CZ	-5.80	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	LEU	C-N	-5.80	1.20	1.34
1	A	91	ARG	NE-CZ	5.76	1.40	1.33
1	A	33	TYR	CD2-CE2	5.69	1.47	1.39
1	A	17	GLY	CA-C	5.66	1.60	1.51
1	A	30	GLU	CD-OE1	5.56	1.31	1.25
1	A	172	GLU	N-CA	5.56	1.57	1.46
1	A	154	GLU	CD-OE2	5.52	1.31	1.25
1	A	81	GLU	CD-OE1	-5.40	1.19	1.25
1	A	57	TRP	C-O	5.37	1.33	1.23
1	A	147	PHE	C-O	5.36	1.33	1.23
1	A	129	GLY	N-CA	5.31	1.54	1.46
1	A	24	TRP	CZ2-CH2	5.23	1.47	1.37
1	A	121	TYR	CD2-CE2	5.22	1.47	1.39
1	A	16	ILE	CA-CB	5.20	1.66	1.54
1	A	176	LYS	N-CA	5.19	1.56	1.46
1	A	114	ILE	C-O	5.18	1.33	1.23
1	A	26	PRO	N-CD	5.15	1.55	1.47
1	A	78	GLU	CD-OE2	5.14	1.31	1.25
1	A	49	LEU	N-CA	5.12	1.56	1.46
1	A	51	ILE	CB-CG2	5.06	1.68	1.52

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	ARG	NE-CZ-NH1	-25.77	107.42	120.30
1	A	145	ASP	CB-CG-OD1	23.16	139.14	118.30
1	A	65	ARG	NE-CZ-NH2	22.10	131.35	120.30
1	A	78	GLU	OE1-CD-OE2	-19.98	99.32	123.30
1	A	77	ARG	NE-CZ-NH2	18.04	129.32	120.30
1	A	141	ASP	CB-CG-OD2	15.26	132.03	118.30
1	A	121	TYR	CB-CG-CD2	-13.57	112.86	121.00
1	A	141	ASP	CB-CG-OD1	-13.28	106.34	118.30
1	A	110	ASP	CB-CG-OD2	13.25	130.23	118.30
1	A	34	PHE	CB-CG-CD2	-11.87	112.49	120.80
1	A	88	PHE	CB-CG-CD2	11.87	129.11	120.80
1	A	171	GLU	OE1-CD-OE2	11.78	137.43	123.30
1	A	36	ARG	NE-CZ-NH1	11.71	126.16	120.30
1	A	121	TYR	CZ-CE2-CD2	-11.64	109.32	119.80
1	A	28	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	A	145	ASP	OD1-CG-OD2	-10.71	102.96	123.30
1	A	77	ARG	CG-CD-NE	-10.64	89.44	111.80
1	A	70	ARG	NE-CZ-NH2	-10.38	115.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	165	VAL	CG1-CB-CG2	10.20	127.22	110.90
1	A	90	SER	N-CA-CB	10.09	125.63	110.50
1	A	88	PHE	CB-CG-CD1	-9.97	113.82	120.80
1	A	156	TYR	CB-CG-CD2	-9.60	115.24	121.00
1	A	126	ASN	CB-CG-OD1	9.46	140.52	121.60
1	A	10	VAL	CA-CB-CG2	9.46	125.08	110.90
1	A	22	LEU	CB-CG-CD1	9.35	126.89	111.00
1	A	123	GLU	CA-CB-CG	9.31	133.88	113.40
1	A	186	ASP	CB-CG-OD1	9.25	126.62	118.30
1	A	65	ARG	NH1-CZ-NH2	-9.20	109.28	119.40
1	A	31	SER	N-CA-CB	9.06	124.09	110.50
1	A	19	ASN	OD1-CG-ND2	-8.94	101.34	121.90
1	A	53	GLY	CA-C-O	8.94	136.69	120.60
1	A	28	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	95	ASP	CB-CG-OD1	8.84	126.25	118.30
1	A	120	VAL	O-C-N	8.75	136.71	122.70
1	A	182	TYR	CB-CG-CD1	-8.69	115.78	121.00
1	A	172	GLU	OE1-CD-OE2	8.51	133.52	123.30
1	A	109	VAL	O-C-N	8.50	136.30	122.70
1	A	184	LYS	CB-CA-C	-8.46	93.47	110.40
1	A	77	ARG	CD-NE-CZ	-8.20	112.13	123.60
1	A	133	LEU	CA-CB-CG	8.17	134.09	115.30
1	A	22	LEU	CB-CG-CD2	-8.10	97.22	111.00
1	A	108	LYS	CB-CA-C	-7.96	94.48	110.40
1	A	9	ALA	CA-C-N	7.95	134.68	117.20
1	A	185	ASN	N-CA-CB	7.91	124.84	110.60
1	A	93	LEU	CB-CG-CD2	-7.87	97.62	111.00
1	A	101	GLU	CA-CB-CG	7.87	130.72	113.40
1	A	140	GLN	N-CA-CB	7.87	124.77	110.60
1	A	119	SER	N-CA-CB	-7.86	98.71	110.50
1	A	138	ILE	CA-CB-CG1	7.80	125.82	111.00
1	A	44	GLU	O-C-N	7.79	136.44	123.20
1	A	171	GLU	O-C-N	7.77	135.13	122.70
1	A	133	LEU	CB-CG-CD2	7.75	124.18	111.00
1	A	162	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	A	166	LEU	CB-CG-CD1	7.66	124.02	111.00
1	A	172	GLU	CB-CA-C	7.62	125.64	110.40
1	A	19	ASN	CB-CG-ND2	7.59	134.91	116.70
1	A	175	ILE	O-C-N	7.57	134.81	122.70
1	A	32	ARG	O-C-N	-7.55	110.62	122.70
1	A	33	TYR	O-C-N	7.30	134.39	122.70
1	A	32	ARG	NE-CZ-NH2	7.28	123.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	GLY	O-C-N	7.25	134.30	122.70
1	A	54	LYS	CD-CE-NZ	7.23	128.33	111.70
1	A	44	GLU	CA-CB-CG	7.20	129.24	113.40
1	A	6	CYS	N-CA-CB	7.18	123.52	110.60
1	A	110	ASP	O-C-N	-7.16	111.25	122.70
1	A	153	LEU	CB-CG-CD1	-7.14	98.86	111.00
1	A	137	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	A	138	ILE	CB-CG1-CD1	7.11	133.79	113.90
1	A	81	GLU	CA-CB-CG	7.08	128.97	113.40
1	A	9	ALA	C-N-CA	7.04	139.30	121.70
1	A	99	LEU	CA-CB-CG	7.04	131.49	115.30
1	A	18	LYS	O-C-N	-7.03	111.45	122.70
1	A	53	GLY	O-C-N	-7.01	111.48	122.70
1	A	94	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	A	113	TRP	CZ3-CH2-CZ2	6.96	129.95	121.60
1	A	128	PRO	C-N-CA	-6.89	107.83	122.30
1	A	74	VAL	CA-CB-CG2	6.88	121.23	110.90
1	A	9	ALA	O-C-N	-6.85	111.74	122.70
1	A	134	PHE	N-CA-CB	6.83	122.90	110.60
1	A	181	VAL	O-C-N	-6.82	111.79	122.70
1	A	113	TRP	CH2-CZ2-CE2	-6.77	110.63	117.40
1	A	113	TRP	CE3-CZ3-CH2	-6.75	113.77	121.20
1	A	32	ARG	CD-NE-CZ	6.74	133.03	123.60
1	A	121	TYR	CE1-CZ-CE2	6.73	130.57	119.80
1	A	28	ARG	N-CA-CB	6.73	122.71	110.60
1	A	21	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	110	ASP	CB-CG-OD1	-6.70	112.27	118.30
1	A	65	ARG	CD-NE-CZ	6.68	132.96	123.60
1	A	162	TYR	CG-CD2-CE2	-6.67	115.96	121.30
1	A	182	TYR	CZ-CE2-CD2	-6.64	113.82	119.80
1	A	112	VAL	CA-CB-CG1	-6.63	100.95	110.90
1	A	58	PHE	CB-CG-CD1	-6.62	116.17	120.80
1	A	179	PHE	CA-C-N	6.57	131.64	117.20
1	A	173	LYS	CD-CE-NZ	-6.56	96.61	111.70
1	A	166	LEU	CB-CG-CD2	-6.55	99.87	111.00
1	A	172	GLU	CG-CD-OE2	-6.52	105.26	118.30
1	A	140	GLN	O-C-N	6.51	133.11	122.70
1	A	10	VAL	CG1-CB-CG2	-6.45	100.58	110.90
1	A	16	ILE	CA-C-N	6.45	129.10	116.20
1	A	114	ILE	O-C-N	-6.43	112.40	122.70
1	A	168	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	56	THR	CA-CB-OG1	-6.39	95.57	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	44	GLU	CB-CA-C	-6.38	97.63	110.40
1	A	9	ALA	N-CA-CB	6.37	119.02	110.10
1	A	49	LEU	CB-CG-CD2	-6.36	100.18	111.00
1	A	58	PHE	CA-C-O	-6.34	106.78	120.10
1	A	156	TYR	CG-CD1-CE1	-6.34	116.22	121.30
1	A	44	GLU	OE1-CD-OE2	6.33	130.89	123.30
1	A	186	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	78	GLU	CA-CB-CG	6.32	127.30	113.40
1	A	86	ALA	N-CA-CB	6.31	118.93	110.10
1	A	154	GLU	CG-CD-OE2	-6.31	105.69	118.30
1	A	182	TYR	CD1-CE1-CZ	-6.28	114.15	119.80
1	A	101	GLU	CG-CD-OE1	6.27	130.84	118.30
1	A	58	PHE	O-C-N	6.26	132.72	122.70
1	A	148	PHE	CB-CG-CD1	6.25	125.17	120.80
1	A	173	LYS	CB-CA-C	-6.23	97.94	110.40
1	A	25	PRO	CB-CA-C	6.23	127.57	112.00
1	A	78	GLU	CG-CD-OE1	6.22	130.75	118.30
1	A	128	PRO	CA-C-O	6.21	135.10	120.20
1	A	31	SER	CB-CA-C	-6.18	98.35	110.10
1	A	44	GLU	CA-C-O	-6.18	107.12	120.10
1	A	123	GLU	N-CA-CB	-6.18	99.48	110.60
1	A	36	ARG	CG-CD-NE	6.17	124.76	111.80
1	A	126	ASN	O-C-N	-6.14	112.87	122.70
1	A	44	GLU	CG-CD-OE2	-6.09	106.12	118.30
1	A	183	GLU	CG-CD-OE2	6.09	130.47	118.30
1	A	125	MET	CA-CB-CG	-6.04	103.04	113.30
1	A	27	LEU	CA-C-O	-6.01	107.48	120.10
1	A	182	TYR	CD1-CG-CD2	6.00	124.49	117.90
1	A	175	ILE	C-N-CA	-5.99	106.73	121.70
1	A	42	SER	CA-C-O	-5.98	107.53	120.10
1	A	168	ASP	OD1-CG-OD2	-5.97	111.95	123.30
1	A	31	SER	CA-CB-OG	-5.96	95.10	111.20
1	A	49	LEU	CB-CG-CD1	-5.96	100.87	111.00
1	A	91	ARG	CG-CD-NE	-5.95	99.31	111.80
1	A	142	PHE	N-CA-CB	5.94	121.29	110.60
1	A	111	MET	CA-CB-CG	-5.92	103.23	113.30
1	A	171	GLU	C-N-CA	-5.91	106.93	121.70
1	A	77	ARG	CA-CB-CG	-5.91	100.40	113.40
1	A	37	MET	CG-SD-CE	5.87	109.59	100.20
1	A	94	ASP	OD1-CG-OD2	5.84	134.39	123.30
1	A	119	SER	O-C-N	-5.79	113.44	122.70
1	A	168	ASP	CB-CG-OD2	5.78	123.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	81	GLU	CG-CD-OE1	5.74	129.78	118.30
1	A	137	ARG	N-CA-CB	5.73	120.92	110.60
1	A	47	GLN	CB-CA-C	-5.73	98.95	110.40
1	A	109	VAL	CA-CB-CG2	5.71	119.47	110.90
1	A	101	GLU	CB-CA-C	-5.68	99.04	110.40
1	A	164	GLY	O-C-N	-5.67	113.63	122.70
1	A	9	ALA	CB-CA-C	5.66	118.59	110.10
1	A	13	ASN	CB-CG-OD1	5.65	132.91	121.60
1	A	17	GLY	N-CA-C	-5.64	99.00	113.10
1	A	174	GLY	O-C-N	5.64	131.73	122.70
1	A	146	THR	O-C-N	5.61	131.68	122.70
1	A	128	PRO	CB-CA-C	5.59	125.98	112.00
1	A	148	PHE	CG-CD1-CE1	5.59	126.95	120.80
1	A	166	LEU	O-C-N	-5.58	113.77	122.70
1	A	152	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	126	ASN	CB-CA-C	5.58	121.55	110.40
1	A	156	TYR	CG-CD2-CE2	-5.57	116.84	121.30
1	A	167	SER	CA-CB-OG	-5.57	96.16	111.20
1	A	95	ASP	O-C-N	5.56	131.59	122.70
1	A	113	TRP	NE1-CE2-CZ2	-5.55	124.30	130.40
1	A	36	ARG	NH1-CZ-NH2	-5.55	113.30	119.40
1	A	89	LEU	CB-CG-CD2	-5.54	101.58	111.00
1	A	81	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	A	13	ASN	OD1-CG-ND2	-5.51	109.22	121.90
1	A	95	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	87	HIS	CE1-NE2-CD2	5.49	120.33	106.60
1	A	138	ILE	CA-C-O	5.49	131.62	120.10
1	A	128	PRO	CA-C-N	-5.47	105.26	116.20
1	A	34	PHE	CG-CD2-CE2	-5.44	114.82	120.80
1	A	25	PRO	N-CA-CB	-5.42	96.64	102.60
1	A	70	ARG	CA-C-O	-5.41	108.73	120.10
1	A	14	MET	CG-SD-CE	5.41	108.86	100.20
1	A	78	GLU	CG-CD-OE2	5.41	129.12	118.30
1	A	54	LYS	N-CA-CB	-5.39	100.90	110.60
1	A	157	LYS	CA-CB-CG	-5.37	101.59	113.40
1	A	70	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	133	LEU	CB-CG-CD1	5.36	120.11	111.00
1	A	101	GLU	OE1-CD-OE2	-5.35	116.88	123.30
1	A	87	HIS	ND1-CE1-NE2	-5.35	98.13	109.90
1	A	91	ARG	CA-CB-CG	-5.29	101.75	113.40
1	A	165	VAL	CA-CB-CG2	-5.28	102.97	110.90
1	A	126	ASN	C-N-CA	5.27	134.87	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	159	LEU	CB-CG-CD2	5.27	119.95	111.00
1	A	94	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	A	138	ILE	N-CA-C	-5.26	96.80	111.00
1	A	169	VAL	CA-CB-CG2	5.25	118.77	110.90
1	A	96	ALA	CB-CA-C	5.24	117.95	110.10
1	A	41	SER	N-CA-CB	5.22	118.33	110.50
1	A	171	GLU	CG-CD-OE1	-5.21	107.88	118.30
1	A	154	GLU	OE1-CD-OE2	5.20	129.54	123.30
1	A	74	VAL	CG1-CB-CG2	-5.17	102.62	110.90
1	A	58	PHE	CZ-CE2-CD2	-5.17	113.89	120.10
1	A	52	MET	O-C-N	5.16	131.97	123.20
1	A	91	ARG	CD-NE-CZ	5.15	130.81	123.60
1	A	35	GLN	OE1-CD-NE2	-5.14	110.08	121.90
1	A	126	ASN	OD1-CG-ND2	-5.14	110.09	121.90
1	A	101	GLU	CB-CG-CD	5.12	128.03	114.20
1	A	11	SER	CB-CA-C	5.12	119.83	110.10
1	A	143	GLU	N-CA-CB	-5.12	101.39	110.60
1	A	59	SER	CA-C-N	5.11	128.43	117.20
1	A	75	LEU	N-CA-CB	5.10	120.59	110.40
1	A	114	ILE	CA-C-N	5.06	128.34	117.20
1	A	146	THR	CA-C-O	-5.03	109.54	120.10
1	A	44	GLU	C-N-CA	-5.00	111.79	122.30

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 (i)

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	71	0
2	A	48	0	26	2	0
3	A	32	0	20	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	51	0	0	3	0
All	All	1628	0	1552	71	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 23.

All (71) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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:28:ARG:HG3	4:A:203:HOH:O	1.66	0.93
1:A:99:LEU:HD22	1:A:105:LEU:HD12	1.51	0.91
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: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:125:MET:HE3	1:A:148:PHE:HZ	1.51	0.73
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:HE2	1:A:133:LEU:HD11	1.76	0.67
1:A:36:ARG:NH1	1:A:37:MET:HE1	2.11	0.64
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:125:MET:HE2	1:A:133:LEU:HD21	1.81	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:125:MET:HE2	1:A:133:LEU:CD1	2.31	0.61
1:A:99:LEU:CD2	1:A:105:LEU:HD12	2.29	0.59
1:A:72:ASN:H	1:A:87:HIS:CD2	2.17	0.59
1:A:156:TYR:CZ	1:A:184:LYS:HD3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:MET:HA	1:A:37:MET:HE2	1.85	0.58
1:A:130:HIS:CE1	1:A:183:GLU:HG3	2.38	0.58
1:A:125:MET:HE2	1:A:133:LEU:CD2	2.35	0.57
1:A:105:LEU:O	1:A:108:LYS:HB2	2.07	0.55
1:A:130:HIS:ND1	1:A:184:LYS:O	2.39	0.55
1:A:99:LEU:HD22	1:A:105:LEU:CD1	2.32	0.55
1:A:10:VAL:CG2	1:A:14:MET:HA	2.36	0.55
1:A:125:MET:HE3	1:A:148:PHE:CZ	2.39	0.54
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	0.52
1:A:43:VAL:CG1	1:A:44:GLU:N	2.74	0.50
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:36:ARG:NH1	1:A:37:MET:HE3	2.29	0.47
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:125:MET:CE	1:A:133:LEU:HD21	2.43	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:37:MET:CE	1:A:37:MET:HA	2.45	0.45
1:A:99:LEU:O	1:A:99:LEU:HD23	2.16	0.45
1:A:43:VAL:HG12	1:A:44:GLU:N	2.30	0.45
1:A:40:THR:O	1:A:111:MET:HE1	2.16	0.45
1:A:125:MET:CE	1:A:133:LEU:CD2	2.95	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:HH12	1:A:37:MET:HE1	1.83	0.42
1:A:103:PRO:O	1:A:104:GLU:C	2.57	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:105:LEU:HA	1:A:108:LYS:HD2	2.03	0.41
1:A:125:MET:HE2	1:A:133:LEU:CG	2.50	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 (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%)	155 (92%)	13 (8%)	13 9

All (13) 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	119	SER
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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	87	HIS
1	A	140	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NDP	A	187	-	45,52,52	2.83	25 (55%)	53,80,80	2.74	24 (45%)
3	MOT	A	188	-	25,34,34	3.01	9 (36%)	28,48,48	3.36	14 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	A	187	-	-	8/30/77/77	0/5/5/5
3	MOT	A	188	-	-	2/18/25/25	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	188	MOT	C11-C	-8.17	1.33	1.50
2	A	187	NDP	P2B-O2B	7.95	1.74	1.59
2	A	187	NDP	O4B-C4B	-6.83	1.29	1.45
3	A	188	MOT	C2-N3	-5.99	1.24	1.35
3	A	188	MOT	C2-NA2	5.55	1.45	1.33
3	A	188	MOT	C9-N10	5.47	1.57	1.46
2	A	187	NDP	C4A-N3A	4.90	1.42	1.35
2	A	187	NDP	O3B-C3B	4.73	1.54	1.43
2	A	187	NDP	C3B-C4B	4.32	1.64	1.53
2	A	187	NDP	C5A-C4A	-3.72	1.31	1.40
2	A	187	NDP	O4D-C1D	3.61	1.50	1.42
2	A	187	NDP	C6A-C5A	3.53	1.56	1.43
3	A	188	MOT	CB-CA	3.52	1.57	1.53
2	A	187	NDP	C3D-C4D	3.46	1.61	1.53
3	A	188	MOT	CM-N10	3.31	1.51	1.46
2	A	187	NDP	C6N-C5N	3.16	1.39	1.33
2	A	187	NDP	PN-O2N	-3.13	1.40	1.55
2	A	187	NDP	PA-O2A	-3.09	1.40	1.55
2	A	187	NDP	O4D-C4D	2.99	1.51	1.45
3	A	188	MOT	C13-C14	-2.94	1.33	1.39
2	A	187	NDP	C6N-N1N	2.84	1.44	1.37
2	A	187	NDP	C7N-C3N	2.81	1.54	1.48
2	A	187	NDP	O4B-C1B	2.65	1.44	1.41
2	A	187	NDP	C2A-N3A	2.45	1.36	1.32
2	A	187	NDP	C3B-C2B	2.42	1.58	1.52
2	A	187	NDP	C8A-N7A	-2.33	1.30	1.34
2	A	187	NDP	C5D-C4D	2.28	1.58	1.51
3	A	188	MOT	CA-N	2.27	1.49	1.46
2	A	187	NDP	PN-O1N	-2.26	1.42	1.50
2	A	187	NDP	PA-O5B	2.25	1.68	1.59
3	A	188	MOT	C6-C4A	2.20	1.44	1.41
2	A	187	NDP	P2B-O2X	-2.10	1.46	1.54
2	A	187	NDP	C1D-N1N	2.09	1.52	1.46
2	A	187	NDP	C5B-C4B	2.08	1.58	1.51

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	188	MOT	CB-CA-N	-7.09	99.88	110.19
2	A	187	NDP	O7N-C7N-C3N	-7.04	107.64	120.90
3	A	188	MOT	C6-C9-N10	-6.84	104.21	114.44
2	A	187	NDP	C3N-C2N-N1N	-6.63	113.64	123.10
3	A	188	MOT	C13-C14-N10	6.01	130.26	121.62
3	A	188	MOT	NA2-C2-N1	-5.47	108.88	117.79
2	A	187	NDP	C1D-N1N-C2N	-5.32	112.25	121.11
2	A	187	NDP	PN-O5D-C5D	5.19	152.10	121.68
3	A	188	MOT	C2-N1-C8A	-5.04	109.60	115.36
3	A	188	MOT	C16-C15-C14	5.01	126.91	120.32
2	A	187	NDP	O3D-C3D-C2D	4.70	127.04	111.82
3	A	188	MOT	C12-C13-C14	4.67	126.47	120.32
3	A	188	MOT	C15-C14-C13	-4.48	110.05	119.16
2	A	187	NDP	C5A-C6A-N6A	4.45	127.11	120.35
2	A	187	NDP	PN-O3-PA	4.22	147.29	132.83
2	A	187	NDP	O3X-P2B-O1X	4.17	126.99	110.68
2	A	187	NDP	O3D-C3D-C4D	-4.01	99.46	111.05
3	A	188	MOT	CM-N10-C9	-3.82	104.70	114.84
2	A	187	NDP	O4D-C1D-N1N	-3.78	100.67	108.06
2	A	187	NDP	C4A-C5A-N7A	-3.61	105.64	109.40
2	A	187	NDP	C5B-C4B-C3B	-3.38	102.51	115.18
2	A	187	NDP	C2D-C1D-N1N	3.16	121.23	113.30
3	A	188	MOT	CM-N10-C14	3.06	124.86	119.57
2	A	187	NDP	O2X-P2B-O2B	-2.84	93.27	105.99
3	A	188	MOT	C16-C11-C12	-2.76	114.65	118.59
2	A	187	NDP	C3B-C2B-C1B	-2.72	97.77	102.89
2	A	187	NDP	C3N-C7N-N7N	2.72	122.49	117.67
2	A	187	NDP	O2A-PA-O1A	2.69	125.55	112.24
2	A	187	NDP	O2B-C2B-C1B	-2.69	100.42	110.10
2	A	187	NDP	O4B-C1B-C2B	-2.68	101.95	106.59
2	A	187	NDP	O5B-C5B-C4B	-2.67	99.79	108.99
2	A	187	NDP	O5D-PN-O1N	2.67	119.49	109.07
2	A	187	NDP	O7N-C7N-N7N	2.56	128.87	122.88
2	A	187	NDP	C5D-C4D-C3D	-2.47	105.91	115.18
3	A	188	MOT	NA2-C2-N3	2.41	120.99	117.25
3	A	188	MOT	C16-C11-C	2.25	127.92	120.62
2	A	187	NDP	O5D-C5D-C4D	-2.13	101.64	108.99
3	A	188	MOT	N1-C2-N3	2.11	130.04	127.22

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	187	NDP	C5D-O5D-PN-O3
2	A	187	NDP	C5D-O5D-PN-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
3	A	188	MOT	CA-CB-CG-CD
2	A	187	NDP	C2B-O2B-P2B-O3X
3	A	188	MOT	CT-CA-N-C
2	A	187	NDP	O4D-C1D-N1N-C2N
2	A	187	NDP	C2D-C1D-N1N-C2N

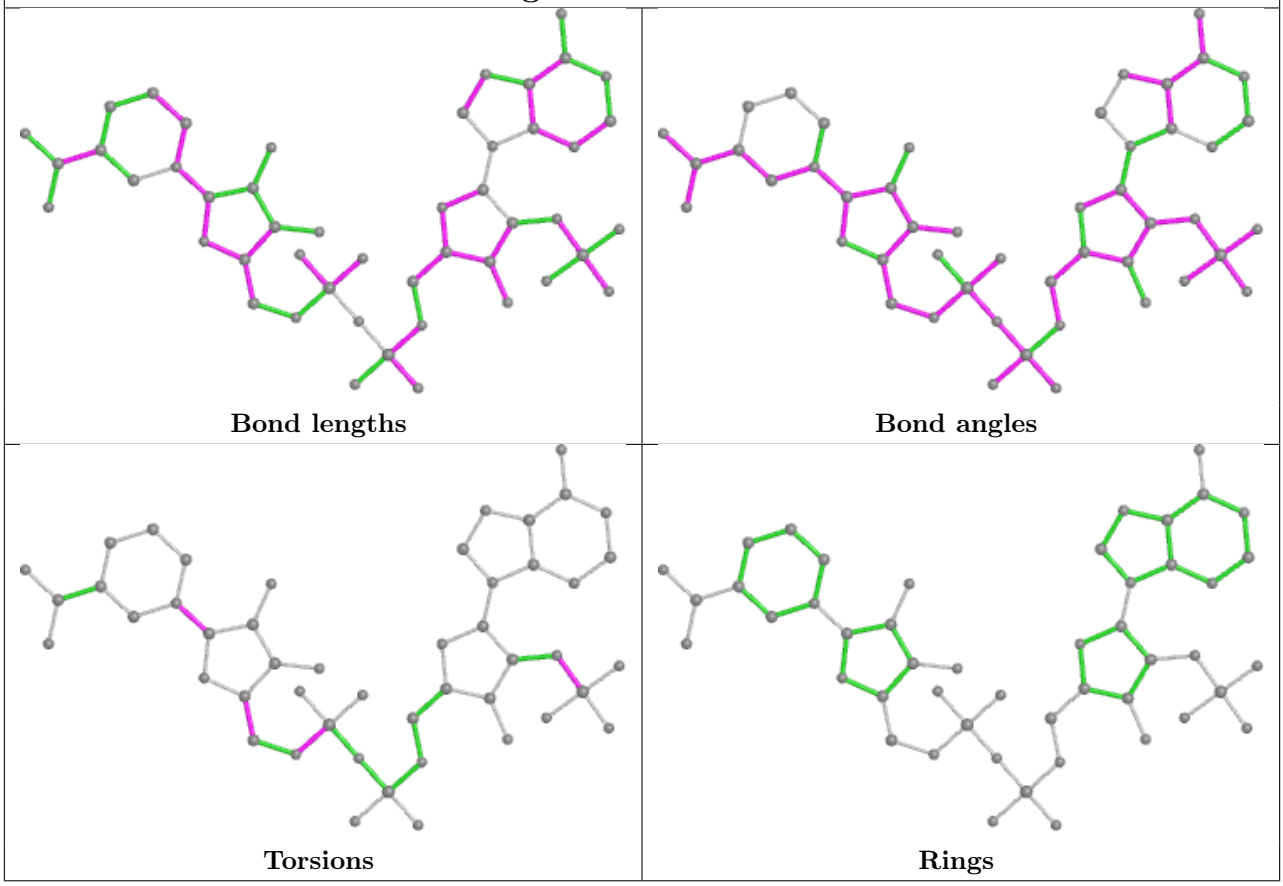
There are no ring outliers.

2 monomers are involved in 4 short contacts:

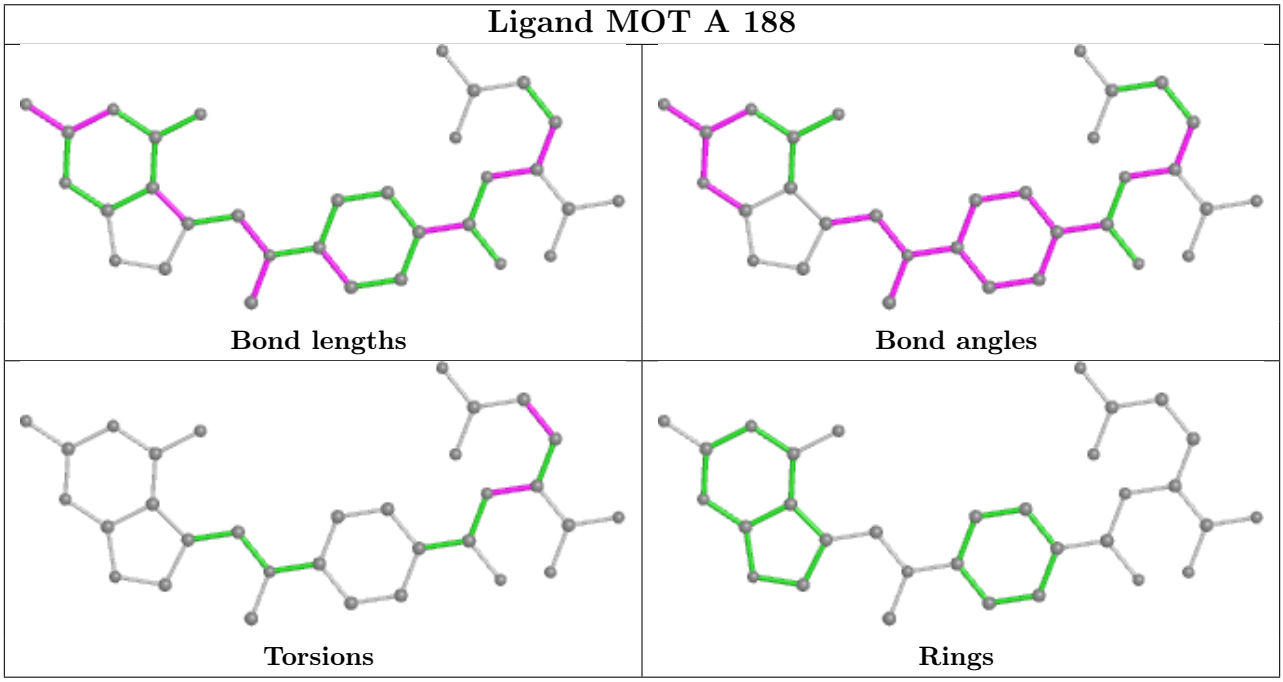
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	187	NDP	2	0
3	A	188	MOT	2	0

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 then 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 NDP A 187



Ligand MOT A 188



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.