



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:49 PM GMT

PDB ID : 1HFP
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

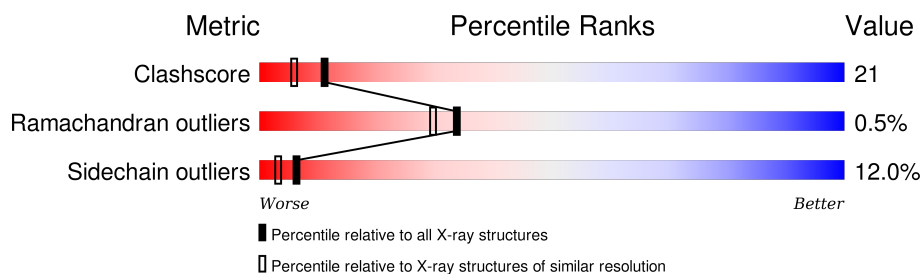
1 Overall quality at a glance

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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	186	<div>48% 34% 17% .</div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1622 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.

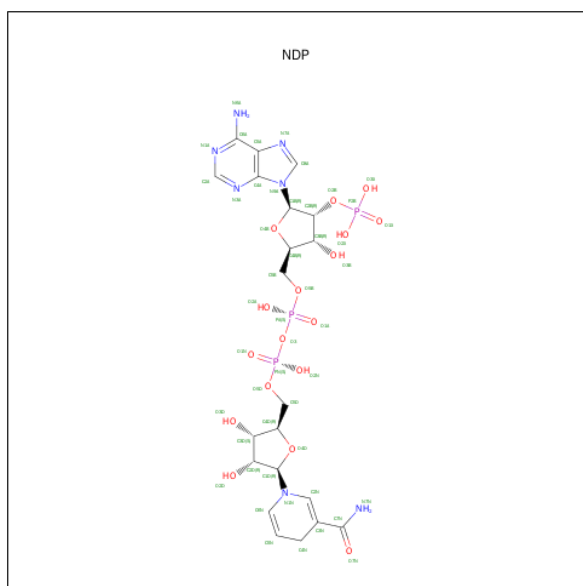
- Molecule 1 is a protein called DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1495	956	253	279	7			

There is a discrepancy between the modelled and reference sequences:

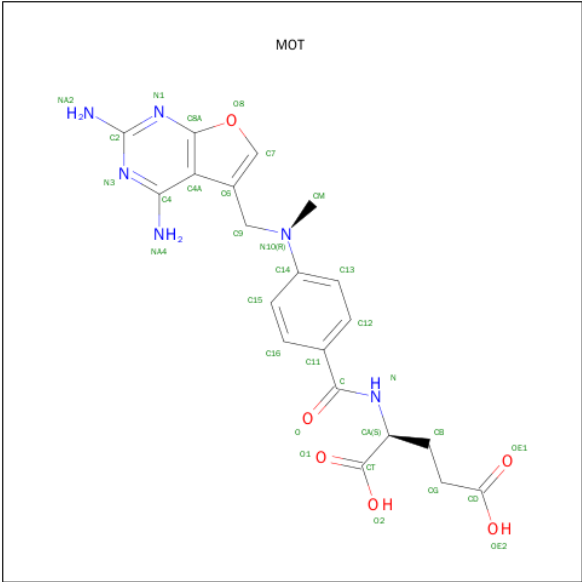
Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLY	PHE	ENGINEERED	UNP P00374

- 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	0	0
			32	20	6	6		

- Molecule 4 is water.

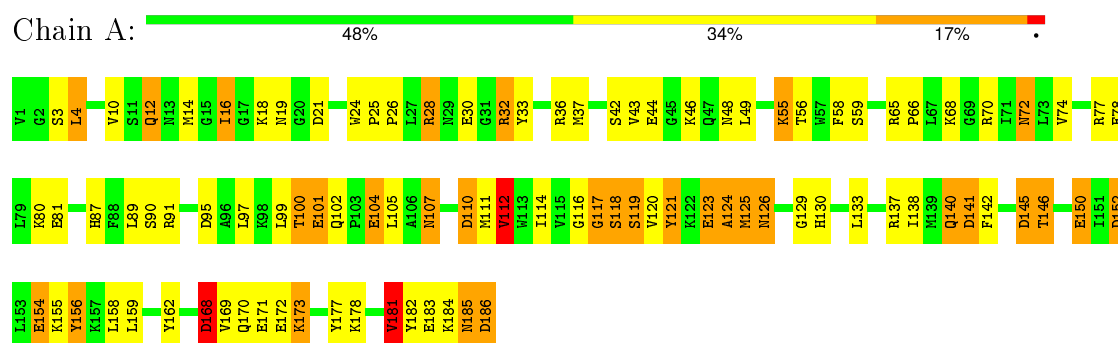
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 will therefore be 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}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1622	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, MOT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.18	4/1529 (0.3%)	2.43	80/2062 (3.9%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	SER	CB-OG	8.07	1.52	1.42
1	A	117	GLY	N-CA	-7.21	1.35	1.46
1	A	78	GLU	CD-OE1	6.58	1.32	1.25
1	A	77	ARG	NE-CZ	5.58	1.40	1.33

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	GLY	C-N-CA	27.36	179.75	122.30
1	A	32	ARG	NE-CZ-NH1	-13.89	113.36	120.30
1	A	145	ASP	CB-CG-OD1	13.61	130.55	118.30
1	A	70	ARG	NE-CZ-NH2	-13.40	113.60	120.30
1	A	168	ASP	CB-CG-OD2	11.71	128.84	118.30
1	A	91	ARG	NE-CZ-NH2	11.61	126.11	120.30
1	A	65	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	A	33	TYR	CB-CG-CD1	-11.12	114.33	121.00
1	A	168	ASP	CB-CG-OD1	-10.43	108.91	118.30
1	A	77	ARG	CG-CD-NE	10.16	133.14	111.80
1	A	77	ARG	CD-NE-CZ	-10.14	109.40	123.60
1	A	70	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	A	77	ARG	NE-CZ-NH2	9.21	124.91	120.30
1	A	182	TYR	CB-CG-CD2	-9.04	115.57	121.00
1	A	33	TYR	CB-CG-CD2	8.94	126.36	121.00
1	A	181	VAL	CA-CB-CG2	8.90	124.25	110.90
1	A	162	TYR	CB-CG-CD1	-8.76	115.74	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	LEU	CA-CB-CG	8.68	135.26	115.30
1	A	141	ASP	CB-CG-OD1	-8.55	110.60	118.30
1	A	140	GLN	N-CA-CB	8.55	125.99	110.60
1	A	172	GLU	CA-CB-CG	8.08	131.18	113.40
1	A	162	TYR	CB-CG-CD2	7.84	125.70	121.00
1	A	58	PHE	CB-CG-CD2	-7.80	115.34	120.80
1	A	156	TYR	CB-CG-CD2	-7.77	116.34	121.00
1	A	141	ASP	CB-CG-OD2	7.75	125.28	118.30
1	A	65	ARG	CD-NE-CZ	7.75	134.45	123.60
1	A	65	ARG	NH1-CZ-NH2	-7.63	111.01	119.40
1	A	4	LEU	CB-CG-CD2	-7.58	98.11	111.00
1	A	101	GLU	CA-CB-CG	7.55	130.01	113.40
1	A	138	ILE	CB-CG1-CD1	7.30	134.33	113.90
1	A	124	ALA	N-CA-CB	6.87	119.72	110.10
1	A	95	ASP	CB-CG-OD1	6.84	124.45	118.30
1	A	126	ASN	CA-CB-CG	6.83	128.42	113.40
1	A	121	TYR	CD1-CE1-CZ	-6.74	113.74	119.80
1	A	158	LEU	CB-CG-CD2	6.71	122.40	111.00
1	A	81	GLU	CG-CD-OE1	6.65	131.60	118.30
1	A	112	VAL	CA-CB-CG1	6.65	120.88	110.90
1	A	90	SER	N-CA-CB	6.58	120.38	110.50
1	A	171	GLU	O-C-N	6.50	133.10	122.70
1	A	32	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	A	126	ASN	CB-CG-OD1	6.39	134.38	121.60
1	A	91	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	A	182	TYR	CB-CG-CD1	6.03	124.62	121.00
1	A	154	GLU	OE1-CD-OE2	6.00	130.50	123.30
1	A	169	VAL	CA-CB-CG2	5.99	119.89	110.90
1	A	12	GLN	CA-CB-CG	-5.98	100.25	113.40
1	A	56	THR	CA-CB-OG1	-5.95	96.50	109.00
1	A	110	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	173	LYS	O-C-N	5.85	133.15	123.20
1	A	30	GLU	CG-CD-OE2	5.83	129.96	118.30
1	A	186	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	177	TYR	CA-CB-CG	5.76	124.35	113.40
1	A	154	GLU	N-CA-CB	5.72	120.89	110.60
1	A	172	GLU	CG-CD-OE2	-5.71	106.87	118.30
1	A	91	ARG	CG-CD-NE	5.71	123.78	111.80
1	A	172	GLU	CG-CD-OE1	5.71	129.72	118.30
1	A	150	GLU	CG-CD-OE2	5.66	129.62	118.30
1	A	74	VAL	CA-CB-CG1	5.63	119.35	110.90
1	A	49	LEU	CB-CG-CD2	-5.60	101.49	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	81	GLU	CA-CB-CG	5.58	125.69	113.40
1	A	55	LYS	CD-CE-NZ	-5.57	98.89	111.70
1	A	158	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	16	ILE	CA-C-N	5.49	127.17	116.20
1	A	59	SER	O-C-N	-5.43	114.01	122.70
1	A	133	LEU	CB-CG-CD1	5.41	120.19	111.00
1	A	138	ILE	CA-CB-CG1	5.37	121.21	111.00
1	A	77	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
1	A	123	GLU	N-CA-CB	-5.30	101.07	110.60
1	A	101	GLU	CB-CA-C	-5.26	99.87	110.40
1	A	65	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	A	137	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	44	GLU	CA-C-O	5.10	130.82	120.10
1	A	19	ASN	OD1-CG-ND2	-5.07	110.23	121.90
1	A	152	ASP	N-CA-CB	-5.07	101.47	110.60
1	A	118	SER	C-N-CA	5.06	134.34	121.70
1	A	154	GLU	CG-CD-OE1	-5.06	108.19	118.30
1	A	141	ASP	CA-CB-CG	-5.04	102.31	113.40
1	A	116	GLY	N-CA-C	5.03	125.68	113.10
1	A	119	SER	N-CA-CB	-5.02	102.97	110.50

There are no chirality outliers.

There are no planarity outliers.

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	1495	0	1504	64	1
2	A	48	0	26	4	0
3	A	32	0	20	0	0
4	A	47	0	0	7	2
All	All	1622	0	1550	65	2

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 21.

All (65) 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:55:LYS:HB2	4:A:224:HOH:O	1.54	1.06
1:A:89:LEU:HD13	4:A:234:HOH:O	1.57	1.05
1:A:28:ARG:NE	1:A:32:ARG:NH2	2.11	0.98
1:A:89:LEU:HB2	4:A:234:HOH:O	1.63	0.98
1:A:28:ARG:HE	1:A:32:ARG:CZ	1.78	0.95
1:A:72:ASN:H	1:A:87:HIS:HD2	1.12	0.95
1:A:12:GLN:HB3	1:A:141:ASP:OD1	1.67	0.94
1:A:99:LEU:CD2	1:A:105:LEU:HD12	1.99	0.92
1:A:117:GLY:HA3	2:A:187:NDP:O2A	1.69	0.91
1:A:99:LEU:HD22	1:A:105:LEU:HD12	1.50	0.91
1:A:28:ARG:HE	1:A:32:ARG:NH2	1.67	0.88
1:A:129:GLY:O	1:A:184:LYS:NZ	2.10	0.83
1:A:28:ARG:CD	1:A:32:ARG:NH2	2.46	0.79
1:A:28:ARG:NE	1:A:32:ARG:HH22	1.84	0.75
1:A:145:ASP:OD1	1:A:146:THR:HG22	1.86	0.74
1:A:89:LEU:CD1	4:A:234:HOH:O	2.25	0.74
1:A:99:LEU:HD23	1:A:99:LEU:O	1.91	0.71
2:A:187:NDP:H8A	2:A:187:NDP:H52A	1.74	0.70
1:A:36:ARG:NH1	1:A:37:MET:CE	2.55	0.70
1:A:28:ARG:HE	1:A:32:ARG:NH1	1.92	0.68
1:A:72:ASN:H	1:A:87:HIS:CD2	2.04	0.68
1:A:121:TYR:O	1:A:125:MET:HB2	1.96	0.66
1:A:36:ARG:NH1	1:A:37:MET:HE1	2.11	0.64
1:A:130:HIS:ND1	1:A:184:LYS:O	2.30	0.64
1:A:26:PRO:O	1:A:173:LYS:HE3	1.98	0.62
1:A:4:LEU:HD12	1:A:112:VAL:HG22	1.82	0.61
1:A:126:ASN:HB2	4:A:216:HOH:O	2.02	0.60
1:A:130:HIS:HE1	1:A:183:GLU:CG	2.15	0.59
1:A:89:LEU:CG	4:A:234:HOH:O	2.51	0.58
1:A:36:ARG:NH1	1:A:37:MET:HE3	2.18	0.57
1:A:97:LEU:O	1:A:100:THR:HB	2.05	0.57
1:A:99:LEU:HA	1:A:102:GLN:HG2	1.86	0.57
1:A:168:ASP:OD1	1:A:168:ASP:N	2.38	0.56
1:A:99:LEU:HD22	1:A:105:LEU:CD1	2.31	0.54
1:A:107:ASN:ND2	1:A:107:ASN:H	2.04	0.54
1:A:10:VAL:HG22	1:A:14:MET:HA	1.90	0.54
1:A:159:LEU:HD12	1:A:181:VAL:HG22	1.89	0.53
1:A:156:TYR:CZ	1:A:184:LYS:HD3	2.43	0.53
1:A:4:LEU:HD11	1:A:114:ILE:HD11	1.91	0.53
1:A:168:ASP:O	1:A:170:GLN:NE2	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HD11	1:A:114:ILE:CD1	2.40	0.52
1:A:152:ASP:OD2	1:A:155:LYS:HE2	2.11	0.51
1:A:100:THR:HG22	1:A:101:GLU:N	2.26	0.51
1:A:28:ARG:NE	1:A:32:ARG:CZ	2.56	0.50
1:A:156:TYR:OH	1:A:184:LYS:HD3	2.11	0.50
1:A:114:ILE:HD13	1:A:124:ALA:HB2	1.93	0.50
1:A:117:GLY:HA3	2:A:187:NDP:PA	2.52	0.49
1:A:16:ILE:O	2:A:187:NDP:H2N	2.13	0.48
1:A:36:ARG:HH12	1:A:37:MET:HE1	1.75	0.48
1:A:99:LEU:CD2	1:A:105:LEU:CD1	2.82	0.48
1:A:130:HIS:CE1	1:A:183:GLU:CG	2.96	0.47
1:A:114:ILE:HD13	1:A:124:ALA:CB	2.45	0.45
1:A:28:ARG:HD2	1:A:32:ARG:NH2	2.28	0.44
1:A:80:LYS:HB3	1:A:80:LYS:HE3	1.71	0.43
1:A:130:HIS:HD1	1:A:185:ASN:HB2	1.84	0.43
1:A:24:TRP:HB2	1:A:25:PRO:HD2	2.01	0.43
1:A:43:VAL:HG11	1:A:46:LYS:HD2	2.00	0.43
1:A:48:ASN:HD21	1:A:111:MET:CE	2.33	0.42
1:A:130:HIS:CE1	1:A:183:GLU:HG3	2.54	0.42
1:A:89:LEU:CB	4:A:234:HOH:O	2.35	0.42
1:A:42:SER:OG	1:A:110:ASP:OD2	2.30	0.42
1:A:186:ASP:OD1	1:A:186:ASP:O	2.37	0.41
1:A:114:ILE:HG23	1:A:120:VAL:HG12	2.03	0.41
1:A:145:ASP:OD1	1:A:146:THR:CG2	2.65	0.40
1:A:140:GLN:HG3	1:A:142:PHE:CE2	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:192:HOH:O	4:A:229:HOH:O[8_544]	2.06	0.14
1:A:154:GLU:OE1	4:A:204:HOH:O[8_544]	2.11	0.09

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%)	178 (97%)	5 (3%)	1 (0%)	34	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/167 (100%)	147 (88%)	20 (12%)	6	3

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

Mol	Chain	Res	Type
1	A	3	SER
1	A	18	LYS
1	A	28	ARG
1	A	66	PRO
1	A	68	LYS
1	A	72	ASN
1	A	100	THR
1	A	104	GLU
1	A	107	ASN
1	A	112	VAL
1	A	118	SER
1	A	119	SER
1	A	123	GLU
1	A	125	MET
1	A	146	THR
1	A	150	GLU
1	A	168	ASP
1	A	178	LYS

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Mol	Chain	Res	Type
1	A	181	VAL
1	A	185	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	48	ASN
1	A	87	HIS
1	A	107	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NDP	A	187	-	42,52,52	2.33	12 (28%)	55,80,80	2.19	18 (32%)
3	MOT	A	188	-	25,34,34	2.27	8 (32%)	26,48,48	3.15	13 (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	-	-	0/30/77/77	0/5/5/5
3	MOT	A	188	-	-	0/18/25/25	0/2/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	O4B-C4B	-8.46	1.25	1.45
3	A	188	MOT	C11-C	-6.39	1.36	1.50
2	A	187	NDP	C5A-C4A	-3.77	1.32	1.40
3	A	188	MOT	C2-N3	-3.67	1.28	1.35
3	A	188	MOT	C4A-C8A	-3.31	1.34	1.42
2	A	187	NDP	O2B-C2B	-3.04	1.34	1.44
2	A	187	NDP	PN-O2N	-2.96	1.42	1.54
2	A	187	NDP	PA-O2A	-2.89	1.42	1.54
3	A	188	MOT	C16-C15	-2.71	1.33	1.38
3	A	188	MOT	C4-N3	-2.34	1.28	1.33
2	A	187	NDP	C4A-N3A	2.28	1.39	1.35
2	A	187	NDP	C3D-C4D	2.39	1.59	1.53
2	A	187	NDP	C1D-N1N	2.58	1.54	1.46
3	A	188	MOT	C9-N10	2.68	1.51	1.47
3	A	188	MOT	C6-C4A	3.22	1.45	1.41
2	A	187	NDP	O3B-C3B	3.42	1.51	1.43
3	A	188	MOT	CB-CA	3.53	1.58	1.53
2	A	187	NDP	C3B-C4B	3.71	1.63	1.53
2	A	187	NDP	O4D-C1D	3.72	1.51	1.42
2	A	187	NDP	P2B-O2B	4.36	1.73	1.60

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188	MOT	C6-C4A-C8A	-7.05	99.47	110.09
3	A	188	MOT	N1-C2-N3	-4.76	120.19	127.44
2	A	187	NDP	C3N-C2N-N1N	-4.09	117.28	123.14
2	A	187	NDP	O4D-C1D-N1N	-3.81	100.02	108.07
3	A	188	MOT	NA2-C2-N1	-3.69	110.73	117.80
3	A	188	MOT	C16-C11-C12	-3.65	113.17	118.60
2	A	187	NDP	O3D-C3D-C4D	-3.50	100.56	111.05
2	A	187	NDP	O4B-C1B-C2B	-3.27	100.68	106.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188	MOT	C15-C14-C13	-2.91	113.08	119.13
2	A	187	NDP	O3B-C3B-C4B	-2.79	102.67	111.05
2	A	187	NDP	O3-PA-O5B	-2.72	95.71	102.94
2	A	187	NDP	O5B-C5B-C4B	-2.65	99.36	109.12
2	A	187	NDP	C1D-N1N-C2N	-2.50	116.55	120.91
3	A	188	MOT	O-C-N	-2.48	117.96	122.44
2	A	187	NDP	C5B-C4B-C3B	-2.36	105.86	115.21
2	A	187	NDP	O5D-C5D-C4D	-2.33	100.52	109.12
3	A	188	MOT	CM-N10-C9	-2.09	108.56	114.23
2	A	187	NDP	C6N-N1N-C2N	2.04	123.77	118.52
3	A	188	MOT	C2-N3-C4	2.30	123.97	116.70
2	A	187	NDP	O2A-PA-O1A	2.46	125.85	112.53
2	A	187	NDP	O3X-P2B-O1X	2.51	118.66	110.58
3	A	188	MOT	C13-C12-C11	2.65	123.83	120.76
2	A	187	NDP	O4B-C1B-N9A	3.20	114.81	108.10
3	A	188	MOT	C13-C14-N10	3.22	126.57	121.68
2	A	187	NDP	O3D-C3D-C2D	3.34	122.69	111.83
2	A	187	NDP	C2D-C1D-N1N	3.77	123.51	113.34
3	A	188	MOT	C16-C15-C14	4.20	125.79	120.36
2	A	187	NDP	PN-O3-PA	4.68	145.87	132.73
3	A	188	MOT	CM-N10-C14	5.26	128.58	119.56
3	A	188	MOT	NA2-C2-N3	7.17	129.07	117.20
2	A	187	NDP	C4B-O4B-C1B	7.40	117.85	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	187	NDP	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.