



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:16 PM GMT

PDB ID : 1S3W  
Title : Structure Determination of TetrahydroquinazolineAntifoaltes in Complex with Human and Pneumocystis carinii Dihydrofolate Reductase: Correlations of Enzyme Selectivity and Stereochemistry  
Authors : Cody, V.; Luft, J.R.; Pangborn, W.; Gangjee, A.; Queener, S.F.  
Deposited on : 2004-01-14  
Resolution : 1.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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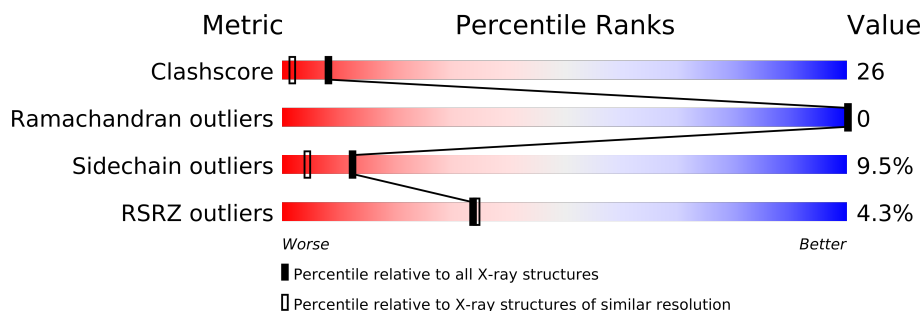
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	186	

## 2 Entry composition i

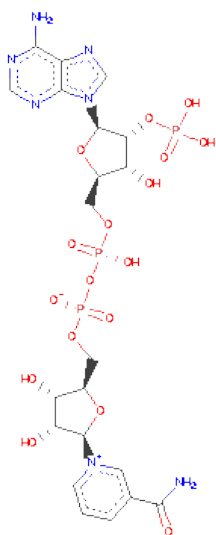
There are 4 unique types of molecules in this entry. The entry contains 1671 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

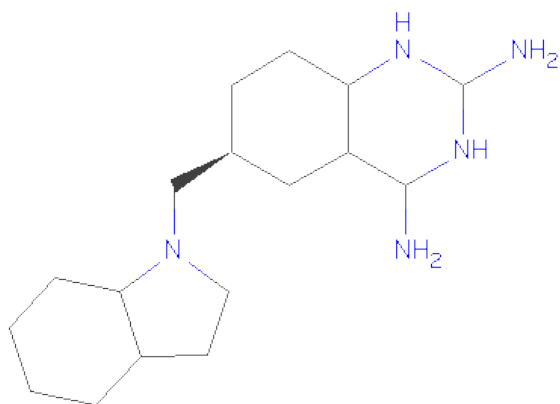
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1509	970	253	279	7	0	1	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0

- Molecule 3 is 6-(OCTAHYDRO-1H-INDOL-1-YLMETHYL)DECAHYDROQUINAZOLIN E-2,4-DIAMINE (three-letter code: TQT) (formula: C<sub>17</sub>H<sub>33</sub>N<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	1
			32	26	6		

- Molecule 4 is water.

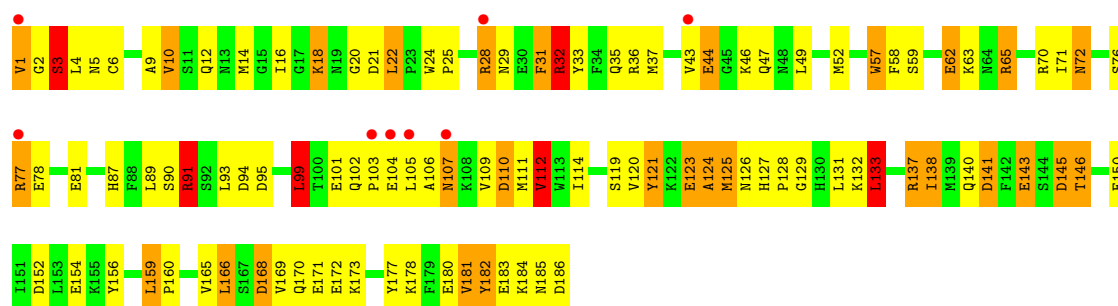
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	82	Total	O	0	0
			82	82		

### 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.

#### ● Molecule 1: Dihydrofolate reductase

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.98Å 86.98Å 76.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.90 43.49 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.90) 64.5 (43.49-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 1.91Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.177 , 0.216 0.192 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.3	EDS
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 10995 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	1671	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	1.19	4/1549 (0.3%)	2.48	86/2089 (4.1%)

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	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	GLU	CD-OE1	-5.77	1.19	1.25
1	A	112	VAL	C-N	5.34	1.46	1.34
1	A	107	ASN	C-N	-5.30	1.21	1.34
1	A	172	GLU	CD-OE1	-5.19	1.20	1.25

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ARG	NE-CZ-NH2	-22.33	109.13	120.30
1	A	65	ARG	NE-CZ-NH2	21.76	131.18	120.30
1	A	65	ARG	CD-NE-CZ	19.96	151.55	123.60
1	A	70	ARG	NE-CZ-NH2	-15.15	112.72	120.30
1	A	137	ARG	NE-CZ-NH2	13.58	127.09	120.30
1	A	137	ARG	NE-CZ-NH1	-13.08	113.76	120.30
1	A	77	ARG	NE-CZ-NH1	12.50	126.55	120.30
1	A	168	ASP	CB-CG-OD1	12.22	129.30	118.30
1	A	70	ARG	NE-CZ-NH1	11.82	126.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	TYR	CB-CG-CD1	-11.49	114.10	121.00
1	A	110	ASP	CB-CG-OD2	-10.40	108.94	118.30
1	A	28	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	A	32	ARG	NE-CZ-NH2	9.09	124.84	120.30
1	A	78	GLU	CA-CB-CG	9.01	133.21	113.40
1	A	145	ASP	CB-CG-OD1	8.96	126.36	118.30
1	A	154	GLU	N-CA-CB	8.74	126.33	110.60
1	A	177	TYR	CB-CG-CD2	-8.70	115.78	121.00
1	A	110	ASP	CB-CG-OD1	8.68	126.11	118.30
1	A	21	ASP	CB-CG-OD1	8.49	125.94	118.30
1	A	112	VAL	CA-C-N	-8.47	98.56	117.20
1	A	10	VAL	CA-CB-CG1	8.38	123.48	110.90
1	A	138	ILE	CA-CB-CG1	8.36	126.88	111.00
1	A	133	LEU	CA-CB-CG	8.34	134.49	115.30
1	A	91	ARG	CD-NE-CZ	-8.25	112.04	123.60
1	A	36	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	A	182	TYR	CB-CG-CD2	-8.17	116.10	121.00
1	A	65	ARG	NH1-CZ-NH2	-7.91	110.70	119.40
1	A	21	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	A	141	ASP	CB-CG-OD1	7.50	125.05	118.30
1	A	140	GLN	N-CA-CB	7.35	123.84	110.60
1	A	123	GLU	CB-CG-CD	7.27	133.82	114.20
1	A	90	SER	N-CA-CB	7.25	121.38	110.50
1	A	152	ASP	CB-CG-OD1	7.25	124.83	118.30
1	A	91	ARG	NH1-CZ-NH2	7.15	127.27	119.40
1	A	94	ASP	CB-CG-OD2	-7.13	111.89	118.30
1	A	182	TYR	CD1-CE1-CZ	-6.95	113.55	119.80
1	A	143	GLU	OE1-CD-OE2	-6.91	115.01	123.30
1	A	181	VAL	CB-CA-C	6.69	124.10	111.40
1	A	1	VAL	CA-CB-CG1	6.64	120.86	110.90
1	A	70	ARG	CD-NE-CZ	6.61	132.86	123.60
1	A	159	LEU	CB-CG-CD1	-6.54	99.89	111.00
1	A	150	GLU	CB-CG-CD	6.52	131.81	114.20
1	A	101	GLU	CA-CB-CG	6.49	127.68	113.40
1	A	91	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	32	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	A	99	LEU	CA-CB-CG	6.24	129.65	115.30
1	A	124	ALA	N-CA-CB	6.16	118.73	110.10
1	A	154	GLU	OE1-CD-OE2	6.08	130.59	123.30
1	A	9	ALA	N-CA-CB	6.08	118.61	110.10
1	A	181	VAL	CA-CB-CG1	5.94	119.81	110.90
1	A	146	THR	CA-CB-CG2	5.94	120.72	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	LEU	CB-CG-CD1	-5.84	101.07	111.00
1	A	132	LYS	CD-CE-NZ	-5.79	98.37	111.70
1	A	126	ASN	CB-CA-C	5.71	121.82	110.40
1	A	90	SER	O-C-N	5.70	131.83	122.70
1	A	166	LEU	N-CA-CB	-5.66	99.09	110.40
1	A	95	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	138	ILE	CG1-CB-CG2	-5.61	99.07	111.40
1	A	168	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	A	111	MET	CG-SD-CE	5.53	109.05	100.20
1	A	52	MET	CA-CB-CG	-5.51	103.93	113.30
1	A	58	PHE	CB-CG-CD1	-5.50	116.95	120.80
1	A	183	GLU	CG-CD-OE1	5.48	129.27	118.30
1	A	181	VAL	CG1-CB-CG2	5.48	119.67	110.90
1	A	159	LEU	CB-CG-CD2	5.46	120.29	111.00
1	A	138	ILE	CB-CG1-CD1	5.43	129.12	113.90
1	A	62	GLU	CG-CD-OE1	5.38	129.06	118.30
1	A	169	VAL	CA-CB-CG2	5.38	118.97	110.90
1	A	35	GLN	OE1-CD-NE2	-5.30	109.70	121.90
1	A	44	GLU	N-CA-CB	5.27	120.08	110.60
1	A	126	ASN	CB-CG-OD1	5.27	132.14	121.60
1	A	121	TYR	CD1-CG-CD2	5.25	123.68	117.90
1	A	57	TRP	CD1-NE1-CE2	-5.24	104.28	109.00
1	A	143	GLU	CA-CB-CG	5.14	124.72	113.40
1	A	123	GLU	N-CA-CB	-5.11	101.40	110.60
1	A	3	SER	O-C-N	5.11	130.87	122.70
1	A	65	ARG	CB-CA-C	-5.10	100.20	110.40
1	A	62	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	A	36	ARG	CD-NE-CZ	-5.06	116.51	123.60
1	A	171	GLU	OE1-CD-OE2	5.05	129.36	123.30
1	A	31[A]	PHE	CB-CG-CD1	-5.04	117.27	120.80
1	A	31[B]	PHE	CB-CG-CD1	-5.04	117.27	120.80
1	A	182	TYR	CB-CG-CD1	5.03	124.02	121.00
1	A	101	GLU	CG-CD-OE1	5.02	128.34	118.30
1	A	6	CYS	O-C-N	5.02	130.73	122.70
1	A	81	GLU	OE1-CD-OE2	-5.01	117.29	123.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	VAL	Mainchain
1	A	32	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	91	ARG	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1509	0	1516	82	0
2	A	48	0	25	6	0
3	A	32	0	41	4	0
4	A	82	0	0	1	0
All	All	1671	0	1582	84	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (84) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:99:LEU:CD2	1:A:105:LEU:HD12	1.79	1.12
1:A:99:LEU:HD21	1:A:105:LEU:HD12	1.28	1.08
1:A:89:LEU:HD21	1:A:91:ARG:HH22	1.15	1.07
1:A:102:GLN:HB2	1:A:104:GLU:HG2	1.51	0.92
1:A:33:TYR:CE2	1:A:37:MET:HE2	2.06	0.89
1:A:72:ASN:H	1:A:87:HIS:HD2	1.17	0.89
1:A:37:MET:HE1	1:A:165:VAL:HG22	1.56	0.87
1:A:43:VAL:HG13	1:A:46:LYS:HB2	1.58	0.86
1:A:77:ARG:NH2	2:A:187:NAP:N1A	2.25	0.84
1:A:77:ARG:HA	1:A:91:ARG:HD2	1.57	0.84
1:A:22:LEU:HD13	3:A:188[A]:TQT:H'31	1.59	0.84
1:A:33:TYR:HE2	1:A:37:MET:HE2	1.41	0.83
1:A:37:MET:CE	1:A:165:VAL:HG22	2.11	0.80
1:A:76:SER:O	1:A:91:ARG:HD3	1.82	0.79
1:A:114:ILE:HD13	1:A:124:ALA:HB2	1.67	0.76
1:A:4:LEU:HD12	1:A:112:VAL:HG22	1.69	0.75
1:A:99:LEU:HD21	1:A:105:LEU:CD1	2.13	0.74
1:A:77:ARG:HH21	2:A:187:NAP:C6A	2.00	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:ILE:O	2:A:187:NAP:H2N	1.87	0.73
1:A:62:GLU:HG3	1:A:65:ARG:NH1	2.02	0.72
1:A:102:GLN:CB	1:A:104:GLU:HG2	2.21	0.71
1:A:43:VAL:HG11	1:A:110:ASP:HB2	1.72	0.71
1:A:2:GLY:N	1:A:110:ASP:O	2.22	0.71
1:A:47:GLN:O	1:A:109:VAL:HA	1.92	0.69
1:A:114:ILE:HD13	1:A:124:ALA:CB	2.23	0.69
1:A:145:ASP:OD1	1:A:146:THR:HG22	1.93	0.69
1:A:77:ARG:NH2	2:A:187:NAP:C6A	2.56	0.69
1:A:71:ILE:HD12	1:A:109:VAL:HG22	1.75	0.68
1:A:72:ASN:H	1:A:87:HIS:CD2	2.07	0.66
1:A:37:MET:HE1	1:A:165:VAL:CG2	2.26	0.65
1:A:77:ARG:HA	1:A:91:ARG:CD	2.27	0.65
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.79	0.64
1:A:127:HIS:CG	1:A:128:PRO:HD2	2.34	0.63
1:A:12:GLN:HB3	1:A:141:ASP:OD1	2.00	0.62
1:A:137:ARG:HB2	1:A:178:LYS:HG2	1.80	0.62
1:A:103:PRO:HA	1:A:106:ALA:HB3	1.81	0.61
1:A:33:TYR:CE2	1:A:37:MET:CE	2.83	0.61
1:A:43:VAL:CG1	1:A:110:ASP:HB2	2.32	0.59
1:A:43:VAL:HG11	1:A:46:LYS:HD2	1.84	0.59
1:A:121:TYR:O	1:A:125:MET:HB2	2.02	0.59
1:A:62:GLU:HG3	1:A:65:ARG:HH12	1.68	0.58
1:A:131:LEU:HD23	1:A:156:TYR:OH	2.03	0.57
1:A:71:ILE:HD12	1:A:109:VAL:CG2	2.35	0.57
1:A:43:VAL:CG1	1:A:46:LYS:HB2	2.32	0.56
1:A:18:LYS:NZ	1:A:143:GLU:OE2	2.37	0.56
1:A:43:VAL:HG13	1:A:43:VAL:O	2.04	0.56
1:A:31[A]:PHE:CE1	3:A:188[A]:TQT:H'01	2.41	0.55
1:A:57:TRP:CZ2	1:A:65:ARG:HD2	2.41	0.55
1:A:57:TRP:CE2	1:A:65:ARG:HD2	2.42	0.55
3:A:188[A]:TQT:H'01	3:A:188[A]:TQT:H7'2	1.90	0.53
1:A:89:LEU:HD21	1:A:91:ARG:NH2	2.00	0.51
1:A:99:LEU:HD23	1:A:99:LEU:O	2.09	0.51
1:A:129:GLY:O	1:A:184:LYS:NZ	2.35	0.51
1:A:99:LEU:HA	1:A:102:GLN:HG2	1.93	0.51
1:A:168:ASP:O	1:A:170:GLN:NE2	2.30	0.51
1:A:184:LYS:NZ	1:A:186:ASP:OD1	2.44	0.50
1:A:20:GLY:O	1:A:59:SER:HB2	2.11	0.50
1:A:22:LEU:HD13	3:A:188[A]:TQT:C'3	2.37	0.50
1:A:29:ASN:HA	1:A:32:ARG:HG3	1.94	0.50
2:A:187:NAP:H8A	2:A:187:NAP:H52A	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:28:ARG:O	1:A:32:ARG:HG3	2.13	0.48
1:A:127:HIS:CD2	1:A:128:PRO:HD2	2.49	0.48
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.54	0.46
1:A:46:LYS:HE2	1:A:107:ASN:HA	1.98	0.46
1:A:43:VAL:HG11	1:A:46:LYS:CD	2.45	0.45
1:A:99:LEU:C	1:A:99:LEU:HD23	2.36	0.45
1:A:102:GLN:C	1:A:104:GLU:N	2.70	0.45
1:A:24:TRP:CB	1:A:25:PRO:HD2	2.44	0.45
1:A:43:VAL:HG21	1:A:46:LYS:HD2	1.98	0.45
1:A:159:LEU:HA	1:A:160:PRO:HD3	1.77	0.45
1:A:114:ILE:HG23	1:A:120:VAL:HG12	1.98	0.45
1:A:10:VAL:HG22	1:A:14:MET:HA	1.99	0.44
1:A:102:GLN:C	1:A:104:GLU:H	2.21	0.44
1:A:133:LEU:HB2	1:A:182:TYR:HB2	2.00	0.43
1:A:156:TYR:CZ	1:A:184:LYS:HD3	2.54	0.43
1:A:93:LEU:HD23	1:A:123:GLU:HG3	2.00	0.43
1:A:110:ASP:OD2	1:A:110:ASP:C	2.57	0.43
1:A:77:ARG:HH21	2:A:187:NAP:C2A	2.24	0.42
1:A:72:ASN:N	1:A:87:HIS:HD2	1.99	0.42
1:A:2:GLY:CA	1:A:110:ASP:O	2.67	0.42
1:A:173:LYS:HD3	4:A:240:HOH:O	2.19	0.41
1:A:3:SER:HB3	1:A:5:ASN:HD21	1.84	0.41
1:A:102:GLN:O	1:A:104:GLU:N	2.53	0.41
1:A:33:TYR:OH	1:A:37:MET:HE3	2.21	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	185/186 (100%)	179 (97%)	6 (3%)	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	169/168 (101%)	153 (90%)	16 (10%)	12 4

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	3	SER
1	A	18	LYS
1	A	22	LEU
1	A	44	GLU
1	A	63	LYS
1	A	72	ASN
1	A	99	LEU
1	A	112	VAL
1	A	119	SER
1	A	125	MET
1	A	133	LEU
1	A	138	ILE
1	A	166	LEU
1	A	181	VAL
1	A	185	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	87	HIS
1	A	185	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
2	NAP	A	187	-	52,52,52	3.12	23 (44%)	80,80,80	2.65	31 (38%)
3	TQT	A	188[A]	-	10,11,25	6.10	6 (60%)	13,15,36	4.04	10 (76%)
3	TQT	A	188[B]	-	10,11,25	6.02	6 (60%)	13,15,36	3.94	10 (76%)

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	NAP	A	187	-	-	0/35/67/67	0/3/5/5
3	TQT	A	188[A]	-	2/2/3/10	0/0/20/49	0/0/2/4
3	TQT	A	188[B]	-	2/2/3/10	0/0/20/49	0/0/2/4

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	188[A]	TQT	C'6-C'1	-12.32	1.33	1.53
3	A	188[B]	TQT	C'6-C'1	-11.28	1.35	1.53
2	A	187	NAP	C4N-C3N	9.17	1.55	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	188[B]	TQT	C'5-C'6	-8.44	1.33	1.53
2	A	187	NAP	C2N-N1N	8.25	1.45	1.35
2	A	187	NAP	O4B-C4B	-7.92	1.26	1.45
3	A	188[A]	TQT	C'5-C'6	-7.79	1.34	1.53
3	A	188[B]	TQT	C'2-C'1	-7.73	1.34	1.52
3	A	188[A]	TQT	C'2-C'1	-7.50	1.35	1.52
3	A	188[A]	TQT	C'4-C'5	-6.86	1.33	1.53
3	A	188[B]	TQT	C'4-C'5	-6.79	1.33	1.53
3	A	188[B]	TQT	C'3-C'2	-6.20	1.35	1.53
2	A	187	NAP	O4D-C1D	6.05	1.50	1.41
2	A	187	NAP	C5N-C4N	6.04	1.53	1.39
3	A	188[A]	TQT	C'3-C'2	-5.94	1.36	1.53
2	A	187	NAP	P2B-O2B	5.46	1.76	1.59
2	A	187	NAP	C4A-N9A	-4.96	1.30	1.37
2	A	187	NAP	C2N-C3N	-4.31	1.32	1.38
3	A	188[B]	TQT	C'4-C'3	-4.02	1.34	1.51
2	A	187	NAP	C5A-C4A	-3.88	1.31	1.40
2	A	187	NAP	O3B-C3B	3.75	1.52	1.43
3	A	188[A]	TQT	C'4-C'3	-3.74	1.35	1.51
2	A	187	NAP	PN-O1N	-3.14	1.41	1.48
2	A	187	NAP	C3B-C4B	2.96	1.61	1.53
2	A	187	NAP	PA-O2A	-2.72	1.42	1.55
2	A	187	NAP	C5B-C4B	2.61	1.60	1.51
2	A	187	NAP	O7N-C7N	-2.48	1.18	1.24
2	A	187	NAP	PN-O2N	-2.25	1.43	1.48
2	A	187	NAP	C6A-C5A	2.16	1.54	1.42
2	A	187	NAP	P2B-O3X	-2.15	1.46	1.54
2	A	187	NAP	C2B-C1B	2.13	1.56	1.52
2	A	187	NAP	C6N-C5N	-2.09	1.33	1.38
2	A	187	NAP	PA-O5B	2.06	1.68	1.59
2	A	187	NAP	O2D-C2D	-2.05	1.38	1.43
2	A	187	NAP	O4B-C1B	2.03	1.44	1.41

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	187	NAP	O7N-C7N-C3N	-8.03	110.53	119.58
2	A	187	NAP	C5N-C4N-C3N	-7.59	110.47	120.32
2	A	187	NAP	O4D-C1D-N1N	-7.03	100.76	107.95
2	A	187	NAP	O4B-C1B-C2B	-6.22	101.14	106.95
2	A	187	NAP	C2N-C3N-C4N	6.20	125.33	118.31
3	A	188[A]	TQT	C'7-C'6-C'1	6.16	114.50	103.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188[B]	TQT	C'5-C'6-C'1	6.09	121.82	113.40
2	A	187	NAP	C4B-O4B-C1B	5.80	116.05	109.75
3	A	188[A]	TQT	C'2-C'1-C'6	5.62	120.62	113.29
3	A	188[B]	TQT	C'7-C'6-C'1	5.54	113.42	103.85
3	A	188[A]	TQT	C'5-C'6-C'1	5.42	120.89	113.40
2	A	187	NAP	O7N-C7N-N7N	5.00	129.82	122.59
3	A	188[B]	TQT	C'4-C'5-C'6	4.44	118.81	111.92
3	A	188[A]	TQT	C'3-C'4-C'5	4.43	121.29	111.45
3	A	188[A]	TQT	C'4-C'5-C'6	4.42	118.79	111.92
3	A	188[B]	TQT	C'7-C'6-C'5	4.32	124.76	113.94
3	A	188[B]	TQT	C'3-C'4-C'5	4.25	120.88	111.45
3	A	188[A]	TQT	C'7-C'6-C'5	4.20	124.46	113.94
3	A	188[B]	TQT	C'2-C'1-C'6	4.18	118.74	113.29
3	A	188[A]	TQT	C'6-C'1-N'0	4.16	107.18	102.17
2	A	187	NAP	PN-O5D-C5D	4.02	134.15	120.24
3	A	188[B]	TQT	C'6-C'1-N'0	3.92	106.90	102.17
3	A	188[B]	TQT	C'4-C'3-C'2	3.88	120.06	111.45
2	A	187	NAP	O2X-P2B-O1X	3.87	123.10	110.44
3	A	188[B]	TQT	C'2-C'1-N'0	3.79	134.35	115.74
3	A	188[B]	TQT	C'3-C'2-C'1	3.75	119.65	110.53
3	A	188[A]	TQT	C'4-C'3-C'2	3.68	119.62	111.45
2	A	187	NAP	O5D-C5D-C4D	-3.52	96.00	108.94
2	A	187	NAP	O4D-C4D-C5D	3.52	121.93	109.36
2	A	187	NAP	N3A-C2A-N1A	3.45	131.59	128.71
3	A	188[A]	TQT	C'2-C'1-N'0	3.35	132.19	115.74
2	A	187	NAP	O2N-PN-O3	-3.35	99.74	108.79
3	A	188[A]	TQT	C'3-C'2-C'1	3.35	118.68	110.53
2	A	187	NAP	O2X-P2B-O2B	-3.32	97.54	107.09
2	A	187	NAP	O2D-C2D-C3D	-3.01	102.05	111.83
2	A	187	NAP	C5D-C4D-C3D	-2.99	103.22	115.21
2	A	187	NAP	O2B-C2B-C1B	-2.88	99.68	110.36
2	A	187	NAP	O3X-P2B-O2B	-2.86	98.86	107.09
2	A	187	NAP	C6N-C5N-C4N	2.85	123.97	119.44
2	A	187	NAP	C2B-C3B-C4B	-2.82	95.26	101.94
2	A	187	NAP	O5B-C5B-C4B	-2.72	98.94	108.94
2	A	187	NAP	O4B-C1B-N9A	2.70	110.96	108.44
2	A	187	NAP	O3-PN-O1N	2.56	114.95	108.83
2	A	187	NAP	O2A-PA-O1A	2.55	126.46	112.21
2	A	187	NAP	O3D-C3D-C2D	-2.51	103.68	111.83
2	A	187	NAP	C5B-C4B-C3B	-2.50	105.19	115.21
2	A	187	NAP	O3B-C3B-C4B	-2.34	104.17	111.08
2	A	187	NAP	O4B-C4B-C5B	-2.23	101.41	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	187	NAP	C3N-C2N-N1N	-2.19	116.67	120.36
2	A	187	NAP	N6A-C6A-N1A	2.16	123.61	119.36
2	A	187	NAP	O3-PA-O5B	-2.02	94.38	103.41

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	188[A]	TQT	C'6
3	A	188[A]	TQT	C'1
3	A	188[B]	TQT	C'6
3	A	188[B]	TQT	C'1

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	186/186 (100%)	-0.06	8 (4%) 34 34	20, 32, 54, 74	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	LEU	4.0
1	A	103	PRO	3.9
1	A	43	VAL	3.7
1	A	104	GLU	3.0
1	A	1	VAL	2.5
1	A	77	ARG	2.3
1	A	107	ASN	2.1
1	A	28	ARG	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TQT	A	188[A]	16/22	0.12	0.92	21,32,33,34	10
3	TQT	A	188[B]	10/22	0.12	0.76	29,30,31,32	10
2	NAP	A	187	48/48	0.07	-0.55	24,28,41,45	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.