Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:05 PM GMT

PDB ID	:	1S3W
Title	:	Structure Determination of Tetrahydroquinazoline Antifoaltes 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 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 (i) symbol.

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

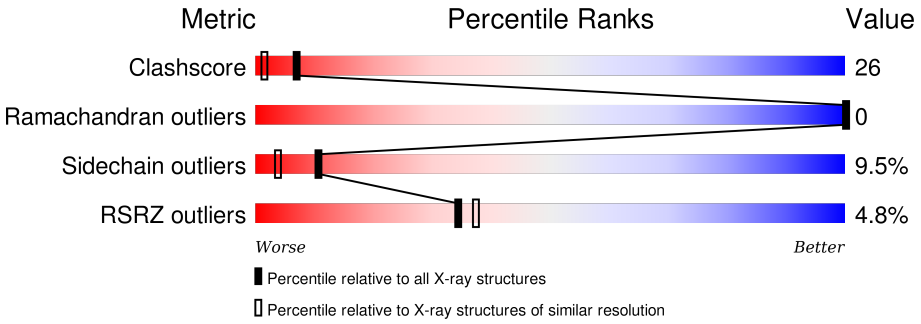
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 >=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 <=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.

Mol	Chain	Length	Quality of chain
1	A	186	5% 42% 39% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TQT	A	188[A]	X	-	-	-
3	TQT	A	188[B]	X	-	-	-

2 Entry composition

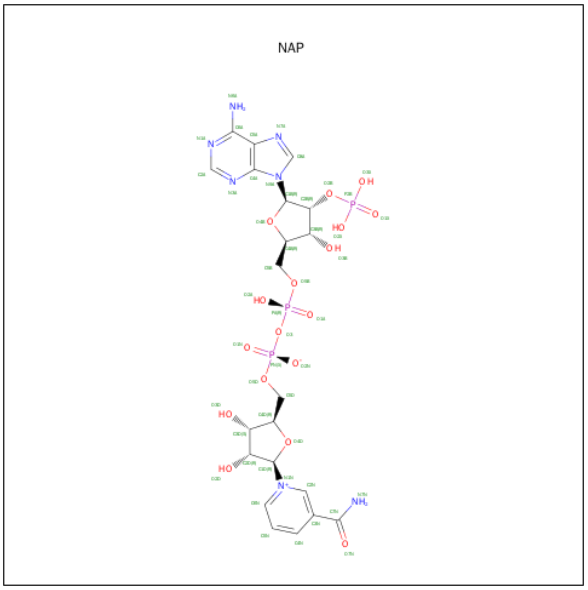
There are 4 unique types of molecules in this entry. The entry contains 1671 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

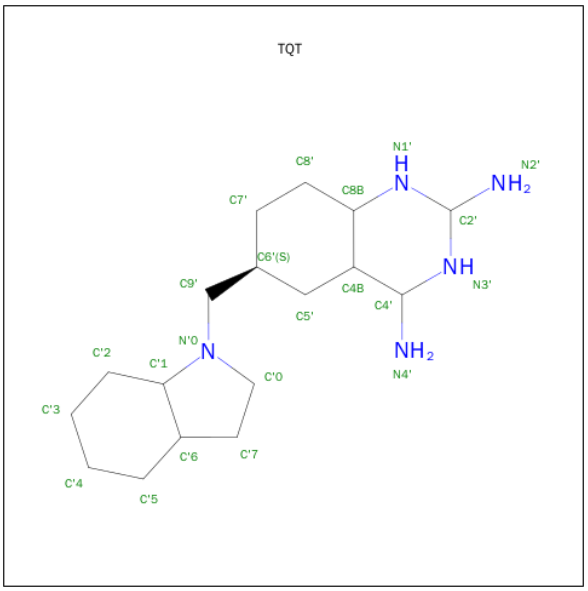
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	1	0
			1509	970	253	279	7			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 3 is 6-(OCTAHYDRO-1H-INDOL-1-YLMETHYL)DECAHYDROQUINAZOLINE-2,4-DIAMINE (three-letter code: TQT) (formula: $C_{17}H_{33}N_5$).



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

- Molecule 4 is water.

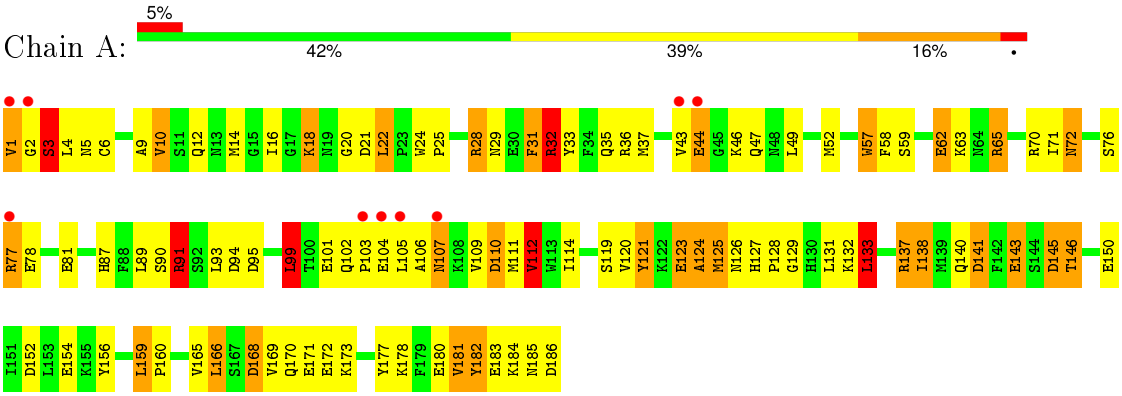
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	82	Total O 82 82	0	0

3 Residue-property plots (i)

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 (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	29.4	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.0	EDS
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 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	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

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 26.

All (84) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:187:NAP:H8A	2:A:187:NAP:H52A	1.95	0.48
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 (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	185/186 (100%)	179 (97%)	6 (3%)	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	169/168 (101%)	153 (90%)	16 (10%)	11 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 molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no 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	-	42,52,52	3.20	20 (47%)	54,80,80	2.98	26 (48%)
3	TQT	A	188[A]	-	21,25,25	6.24	12 (57%)	25,36,36	5.07	16 (64%)
3	TQT	A	188[B]	-	15,15,25	5.21	7 (46%)	16,18,36	4.56	11 (68%)

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	-	-	0/27/67/67	0/5/5/5
3	TQT	A	188[A]	-	2/2/8/10	0/4/49/49	0/4/4/4
3	TQT	A	188[B]	-	2/2/3/10	0/3/23/49	0/2/2/4

All (39) 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	-12.81	1.33	1.53
3	A	188[A]	TQT	C4'-N3'	-12.19	1.26	1.44
3	A	188[B]	TQT	C'6-C'1	-11.73	1.35	1.53
3	A	188[A]	TQT	C8B-N1'	-10.49	1.33	1.47
3	A	188[A]	TQT	C4B-C4'	-9.19	1.35	1.54
3	A	188[B]	TQT	C'5-C'6	-8.68	1.33	1.53
2	A	187	NAP	O4B-C4B	-8.03	1.26	1.45
3	A	188[A]	TQT	C'5-C'6	-8.02	1.34	1.53
3	A	188[B]	TQT	C'2-C'1	-7.92	1.34	1.52
3	A	188[A]	TQT	C'2-C'1	-7.68	1.35	1.52
3	A	188[A]	TQT	C'4-C'5	-7.33	1.33	1.53
3	A	188[A]	TQT	C4B-C8B	-7.28	1.33	1.53
3	A	188[B]	TQT	C'4-C'5	-7.26	1.33	1.53
3	A	188[B]	TQT	C'3-C'2	-6.63	1.35	1.53
3	A	188[A]	TQT	C'3-C'2	-6.34	1.36	1.53
3	A	188[B]	TQT	C'4-C'3	-4.21	1.34	1.51
2	A	187	NAP	C2N-C3N	-4.02	1.32	1.39
3	A	188[A]	TQT	C'4-C'3	-3.92	1.35	1.51
2	A	187	NAP	C5A-C4A	-3.88	1.31	1.40
2	A	187	NAP	PA-O2A	-2.82	1.42	1.54
2	A	187	NAP	PN-O1N	-2.75	1.41	1.51
2	A	187	NAP	O7N-C7N	-2.74	1.18	1.24
2	A	187	NAP	PN-O2N	-2.66	1.43	1.54
3	A	188[B]	TQT	C'1-N'0	-2.23	1.44	1.47
2	A	187	NAP	P2B-O3X	-2.19	1.46	1.54
2	A	187	NAP	C6N-C5N	-2.19	1.33	1.38
2	A	187	NAP	O2D-C2D	-2.06	1.38	1.43
3	A	188[A]	TQT	C'7-C'0	2.00	1.56	1.52
2	A	187	NAP	C6N-N1N	2.03	1.40	1.35
2	A	187	NAP	PA-O5B	2.07	1.68	1.59
3	A	188[A]	TQT	C8'-C7'	2.20	1.58	1.52
2	A	187	NAP	O4B-C1B	2.58	1.44	1.41
2	A	187	NAP	C5B-C4B	2.62	1.60	1.51
2	A	187	NAP	C3B-C4B	3.03	1.61	1.53
2	A	187	NAP	O3B-C3B	3.79	1.52	1.43
2	A	187	NAP	P2B-O2B	5.50	1.76	1.60
2	A	187	NAP	C5N-C4N	6.85	1.53	1.38
2	A	187	NAP	O4D-C1D	7.48	1.50	1.41
2	A	187	NAP	C4N-C3N	9.29	1.55	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	187	NAP	O7N-C7N-C3N	-8.30	110.53	119.59
2	A	187	NAP	C5N-C4N-C3N	-7.85	110.47	120.33
2	A	187	NAP	O4D-C1D-N1N	-6.71	100.76	108.13
2	A	187	NAP	O5D-C5D-C4D	-3.56	96.00	109.12
2	A	187	NAP	O3-PA-O5B	-3.22	94.38	102.94
2	A	187	NAP	C3N-C2N-N1N	-3.21	116.67	120.36
2	A	187	NAP	O4B-C1B-C2B	-3.02	101.14	106.60
2	A	187	NAP	C5D-C4D-C3D	-3.02	103.22	115.21
2	A	187	NAP	O2D-C2D-C3D	-3.01	102.05	111.83
2	A	187	NAP	C2B-C3B-C4B	-2.78	95.26	101.85
2	A	187	NAP	O5B-C5B-C4B	-2.76	98.94	109.12
2	A	187	NAP	O2B-C2B-C1B	-2.65	99.68	110.02
2	A	187	NAP	C5B-C4B-C3B	-2.52	105.19	115.21
2	A	187	NAP	O3D-C3D-C2D	-2.51	103.68	111.83
2	A	187	NAP	O3B-C3B-C4B	-2.29	104.17	111.05
2	A	187	NAP	O4B-C4B-C5B	-2.21	101.41	109.32
2	A	187	NAP	N6A-C6A-N1A	2.05	123.61	119.20
2	A	187	NAP	O2A-PA-O1A	2.57	126.46	112.53
2	A	187	NAP	PN-O3-PA	2.61	140.07	132.73
2	A	187	NAP	C6N-C5N-C4N	2.99	123.97	119.44
3	A	188[A]	TQT	C'0-N'0-C9'	3.13	129.87	112.19
3	A	188[A]	TQT	C'3-C'2-C'1	3.42	118.68	110.38
2	A	187	NAP	O4D-C4D-C5D	3.52	121.93	109.32
2	A	187	NAP	N3A-C2A-N1A	3.53	131.59	128.89
3	A	188[A]	TQT	C4B-C5'-C6'	3.77	112.44	109.31
3	A	188[B]	TQT	C'3-C'2-C'1	3.82	119.65	110.38
2	A	187	NAP	O2X-P2B-O1X	3.89	123.10	110.58
3	A	188[A]	TQT	C'4-C'3-C'2	3.90	119.62	111.44
3	A	188[B]	TQT	C'4-C'3-C'2	4.11	120.06	111.44
3	A	188[A]	TQT	C'7-C'6-C'5	4.13	124.46	113.98
3	A	188[B]	TQT	C'7-C'6-C'5	4.25	124.76	113.98
3	A	188[B]	TQT	C'2-C'1-C'6	4.42	118.74	113.33
3	A	188[A]	TQT	C5'-C4B-C4'	4.43	120.68	112.51
3	A	188[A]	TQT	C'4-C'5-C'6	4.46	118.79	111.92
3	A	188[B]	TQT	C'4-C'5-C'6	4.48	118.81	111.92
3	A	188[B]	TQT	C'3-C'4-C'5	4.50	120.88	111.44
3	A	188[A]	TQT	C'3-C'4-C'5	4.70	121.29	111.44
3	A	188[A]	TQT	C2'-N3'-C4'	4.97	120.79	111.61
3	A	188[B]	TQT	C'0-N'0-C'1	5.00	111.52	104.64
3	A	188[B]	TQT	C'7-C'6-C'1	5.05	113.42	103.73
3	A	188[A]	TQT	C'0-N'0-C'1	5.13	111.70	104.64
2	A	187	NAP	O7N-C7N-N7N	5.13	129.82	122.59
3	A	188[A]	TQT	C'7-C'6-C'1	5.61	114.50	103.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	188[A]	TQT	C'5-C'6-C'1	5.67	120.89	113.45
2	A	187	NAP	C4B-O4B-C1B	5.76	116.05	109.72
3	A	188[A]	TQT	C'2-C'1-C'6	5.95	120.62	113.33
3	A	188[A]	TQT	C8'-C8B-N1'	6.19	116.60	110.89
2	A	187	NAP	C2N-C3N-C4N	6.32	125.33	118.29
3	A	188[B]	TQT	C'5-C'6-C'1	6.38	121.82	113.45
3	A	188[A]	TQT	C'2-C'1-N'0	6.65	132.19	116.65
3	A	188[B]	TQT	C'2-C'1-N'0	7.58	134.35	116.65
3	A	188[B]	TQT	C9'-N'0-C'0	8.45	126.60	113.98
3	A	188[A]	TQT	C8'-C8B-C4B	16.46	126.45	111.05

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.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	187	NAP	6	0
3	A	188[A]	TQT	4	0

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

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^{th} 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^2)	Q<0.9
1	A	186/186 (100%)	-0.11	9 (4%) 34 37	20, 32, 54, 74	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	LEU	4.3
1	A	43	VAL	4.1
1	A	104	GLU	3.2
1	A	1	VAL	3.0
1	A	103	PRO	2.4
1	A	107	ASN	2.3
1	A	2	GLY	2.2
1	A	44	GLU	2.2
1	A	77	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^{th} 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	TQT	A	188[A]	22/22	0.95	0.13	0.68	21,29,33,34	10
3	TQT	A	188[B]	16/22	0.95	0.13	0.56	23,30,31,32	10
2	NAP	A	187	48/48	0.97	0.07	-0.48	24,28,41,45	0

6.5 Other polymers (i)

There are no such residues in this entry.