



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:22 PM GMT

PDB ID : 1TCS  
Title : CRYSTAL STRUCTURE OF TRICHOSANTHIN-NADPH COMPLEX AT 1.7 ANGSTROMS RESOLUTION REVEALS ACTIVE-SITE ARCHITECTURE  
Authors : Xiong, J.-P.; Xia, Z.-X.; Wang, Y.  
Deposited on : 1994-12-27  
Resolution : 1.70 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](mailto: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.

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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 : 1.7 (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

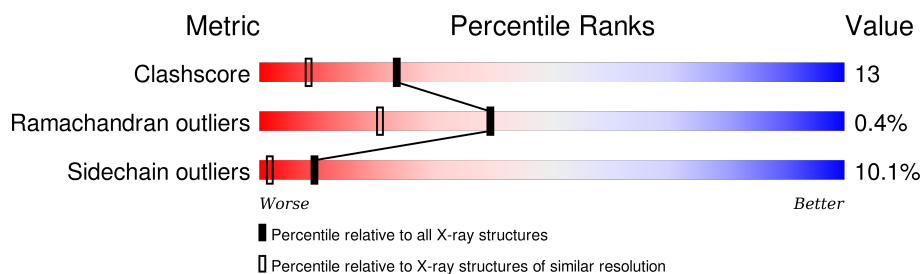
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)

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. 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	247	

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
2	NDP	A	280	X	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2107 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 TRICHOSANTHIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1914	1212	328	370	4			

- 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 water.

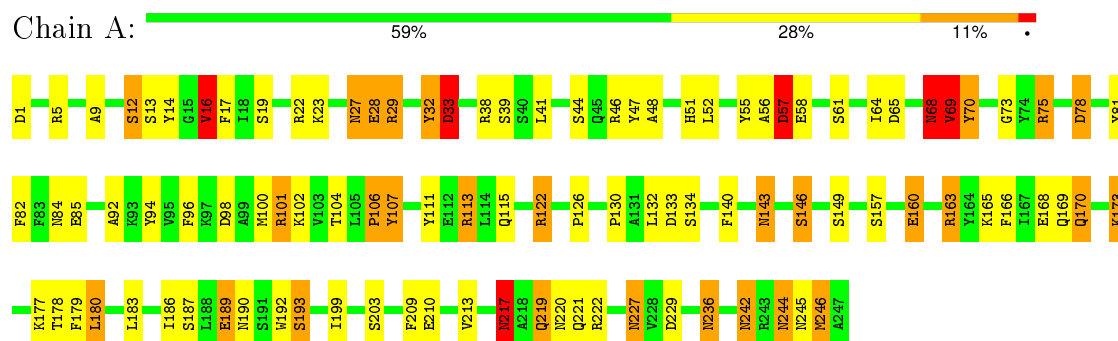
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total	O	0	0
			145	145		

### 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: TRICHOSANTHIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.39Å 76.81Å 79.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, $R_{free}$	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2107	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	1.70	21/1946 (1.1%)	2.60	118/2642 (4.5%)

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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	SER	CA-CB	7.48	1.64	1.52
1	A	58	GLU	CD-OE1	-7.24	1.17	1.25
1	A	73	GLY	N-CA	7.18	1.56	1.46
1	A	189	GLU	CD-OE1	-6.80	1.18	1.25
1	A	19	SER	CB-OG	-6.76	1.33	1.42
1	A	113	ARG	CZ-NH2	6.11	1.41	1.33
1	A	28	GLU	CD-OE2	6.09	1.32	1.25
1	A	222	ARG	CZ-NH1	5.77	1.40	1.33
1	A	160	GLU	CD-OE2	-5.67	1.19	1.25
1	A	130	PRO	N-CA	-5.53	1.37	1.47
1	A	104	THR	CB-OG1	5.43	1.54	1.43
1	A	134	SER	CA-CB	5.27	1.60	1.52
1	A	213	VAL	CB-CG2	5.26	1.64	1.52
1	A	107	TYR	C-O	5.24	1.33	1.23
1	A	12	SER	CA-CB	5.23	1.60	1.52
1	A	23	LYS	C-O	5.22	1.33	1.23
1	A	157	SER	CA-CB	5.17	1.60	1.52
1	A	173	LYS	CA-CB	-5.08	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	GLN	N-CA	5.05	1.56	1.46
1	A	190	ASN	CB-CG	5.04	1.62	1.51
1	A	222	ARG	CZ-NH2	5.03	1.39	1.33

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ARG	NE-CZ-NH1	28.29	134.45	120.30
1	A	113	ARG	NE-CZ-NH1	21.82	131.21	120.30
1	A	101	ARG	NE-CZ-NH1	-21.33	109.64	120.30
1	A	163	ARG	NE-CZ-NH2	18.70	129.65	120.30
1	A	113	ARG	NE-CZ-NH2	-18.66	110.97	120.30
1	A	33	ASP	CB-CG-OD1	-18.55	101.61	118.30
1	A	222	ARG	NE-CZ-NH2	18.21	129.40	120.30
1	A	46	ARG	NH1-CZ-NH2	-13.82	104.19	119.40
1	A	81	TYR	CB-CG-CD2	-13.62	112.83	121.00
1	A	122	ARG	NE-CZ-NH2	-13.51	113.55	120.30
1	A	65	ASP	CB-CG-OD2	-11.63	107.83	118.30
1	A	55	TYR	CB-CG-CD2	-11.40	114.16	121.00
1	A	47	TYR	CB-CG-CD2	11.12	127.67	121.00
1	A	173	LYS	CA-CB-CG	11.10	137.81	113.40
1	A	22	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	A	94	TYR	CB-CG-CD1	-10.84	114.50	121.00
1	A	46	ARG	CD-NE-CZ	10.31	138.04	123.60
1	A	33	ASP	OD1-CG-OD2	9.64	141.62	123.30
1	A	29	ARG	NE-CZ-NH1	9.43	125.01	120.30
1	A	102	LYS	CD-CE-NZ	9.23	132.92	111.70
1	A	55	TYR	CB-CG-CD1	9.09	126.45	121.00
1	A	69	VAL	CG1-CB-CG2	-9.03	96.45	110.90
1	A	222	ARG	NH1-CZ-NH2	-9.02	109.48	119.40
1	A	179	PHE	CB-CG-CD2	-8.96	114.52	120.80
1	A	47	TYR	CB-CG-CD1	-8.69	115.79	121.00
1	A	101	ARG	CD-NE-CZ	-8.31	111.96	123.60
1	A	133	ASP	CB-CG-OD1	8.21	125.69	118.30
1	A	29	ARG	CD-NE-CZ	8.20	135.08	123.60
1	A	14	TYR	CB-CG-CD1	-8.19	116.09	121.00
1	A	82	PHE	CB-CG-CD1	-8.17	115.08	120.80
1	A	101	ARG	NE-CZ-NH2	8.15	124.37	120.30
1	A	122	ARG	NH1-CZ-NH2	7.85	128.04	119.40
1	A	213	VAL	CG1-CB-CG2	-7.75	98.51	110.90
1	A	17	PHE	CB-CG-CD1	-7.64	115.45	120.80
1	A	187	SER	O-C-N	-7.57	110.58	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	TYR	CB-CG-CD1	-7.50	116.50	121.00
1	A	28	GLU	CB-CG-CD	7.47	134.37	114.20
1	A	96	PHE	CB-CG-CD1	7.38	125.96	120.80
1	A	143	ASN	CB-CA-C	7.14	124.67	110.40
1	A	132	LEU	CB-CG-CD2	-7.13	98.88	111.00
1	A	81	TYR	CG-CD2-CE2	-6.92	115.76	121.30
1	A	57	ASP	CB-CG-OD1	-6.90	112.09	118.30
1	A	96	PHE	CB-CG-CD2	-6.89	115.98	120.80
1	A	29	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	75	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	A	16	VAL	CG1-CB-CG2	6.86	121.87	110.90
1	A	168	GLU	CG-CD-OE2	6.74	131.78	118.30
1	A	193	SER	CA-CB-OG	-6.71	93.09	111.20
1	A	146	SER	N-CA-CB	-6.60	100.60	110.50
1	A	58	GLU	CG-CD-OE2	-6.58	105.14	118.30
1	A	28	GLU	CG-CD-OE1	6.53	131.35	118.30
1	A	32	TYR	CG-CD2-CE2	-6.50	116.10	121.30
1	A	210	GLU	CG-CD-OE1	6.50	131.30	118.30
1	A	244	ASN	CB-CG-OD1	-6.49	108.63	121.60
1	A	100	MET	CA-CB-CG	-6.48	102.28	113.30
1	A	13	SER	N-CA-CB	6.43	120.15	110.50
1	A	245	ASN	CB-CA-C	6.42	123.24	110.40
1	A	180	LEU	CB-CG-CD1	6.42	121.91	111.00
1	A	168	GLU	OE1-CD-OE2	-6.38	115.64	123.30
1	A	210	GLU	CG-CD-OE2	-6.32	105.66	118.30
1	A	81	TYR	CB-CG-CD1	6.32	124.79	121.00
1	A	64	ILE	O-C-N	6.31	132.80	122.70
1	A	163	ARG	NE-CZ-NH1	-6.29	117.15	120.30
1	A	65	ASP	OD1-CG-OD2	6.27	135.21	123.30
1	A	57	ASP	OD1-CG-OD2	6.15	134.98	123.30
1	A	246	MET	C-N-CA	6.12	137.01	121.70
1	A	5	ARG	CD-NE-CZ	-6.11	115.04	123.60
1	A	82	PHE	CD1-CE1-CZ	-6.11	112.76	120.10
1	A	85	GLU	OE1-CD-OE2	-6.09	115.99	123.30
1	A	70	TYR	CG-CD1-CE1	6.08	126.16	121.30
1	A	17	PHE	CG-CD1-CE1	-6.05	114.14	120.80
1	A	33	ASP	CA-CB-CG	-6.04	100.12	113.40
1	A	149	SER	CB-CA-C	6.04	121.57	110.10
1	A	57	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	A	173	LYS	CD-CE-NZ	5.99	125.49	111.70
1	A	170	GLN	CG-CD-OE1	5.99	133.58	121.60
1	A	19	SER	CB-CA-C	-5.96	98.77	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ALA	O-C-N	5.93	132.19	122.70
1	A	52	LEU	O-C-N	5.90	132.14	122.70
1	A	68	ASN	O-C-N	5.89	132.12	122.70
1	A	78	ASP	CA-CB-CG	-5.88	100.46	113.40
1	A	101	ARG	NH1-CZ-NH2	5.85	125.84	119.40
1	A	94	TYR	CG-CD1-CE1	-5.84	116.62	121.30
1	A	163	ARG	NH1-CZ-NH2	-5.81	113.01	119.40
1	A	38	ARG	CD-NE-CZ	5.74	131.63	123.60
1	A	82	PHE	CG-CD2-CE2	-5.71	114.52	120.80
1	A	27	ASN	OD1-CG-ND2	-5.68	108.84	121.90
1	A	41	LEU	CB-CG-CD2	-5.66	101.38	111.00
1	A	140	PHE	CB-CG-CD2	-5.61	116.87	120.80
1	A	179	PHE	CD1-CG-CD2	5.57	125.54	118.30
1	A	55	TYR	CD1-CE1-CZ	-5.55	114.80	119.80
1	A	217	ASN	CB-CG-OD1	-5.52	110.56	121.60
1	A	199	ILE	O-C-N	5.48	131.47	122.70
1	A	173	LYS	N-CA-CB	5.47	120.44	110.60
1	A	102	LYS	CB-CG-CD	5.41	125.66	111.60
1	A	48	ALA	O-C-N	5.40	131.34	122.70
1	A	106	PRO	CA-C-O	-5.37	107.31	120.20
1	A	160	GLU	OE1-CD-OE2	-5.36	116.86	123.30
1	A	203	SER	C-N-CA	5.35	135.07	121.70
1	A	75	ARG	NH1-CZ-NH2	-5.33	113.54	119.40
1	A	203	SER	N-CA-CB	5.32	118.48	110.50
1	A	168	GLU	O-C-N	-5.28	114.25	122.70
1	A	143	ASN	N-CA-CB	-5.27	101.11	110.60
1	A	209	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	A	81	TYR	O-C-N	5.22	131.06	122.70
1	A	85	GLU	CG-CD-OE1	5.21	128.71	118.30
1	A	17	PHE	CD1-CG-CD2	5.20	125.05	118.30
1	A	70	TYR	CB-CG-CD1	5.16	124.10	121.00
1	A	170	GLN	O-C-N	-5.16	114.44	122.70
1	A	44	SER	O-C-N	-5.15	114.46	122.70
1	A	222	ARG	CA-C-N	5.15	128.53	117.20
1	A	39	SER	CB-CA-C	5.15	119.88	110.10
1	A	183	LEU	CA-CB-CG	5.11	127.06	115.30
1	A	92	ALA	O-C-N	5.11	130.87	122.70
1	A	38	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	126	PRO	O-C-N	5.10	130.86	122.70
1	A	246	MET	CA-C-N	-5.10	105.99	117.20
1	A	22	ARG	NH1-CZ-NH2	5.05	124.96	119.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	PRO	Mainchain
1	A	113	ARG	Sidechain
1	A	170	GLN	Mainchain

## 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	1914	0	1931	47	0
2	A	48	0	23	25	0
3	A	145	0	0	1	0
All	All	2107	0	1954	52	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 13.

All (52) 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:177:LYS:HG2	1:A:178:THR:N	1.81	0.95
1:A:192:TRP:HB3	2:A:280:NDP:O1A	1.74	0.88
1:A:219:GLN:O	1:A:220:ASN:HB2	1.75	0.86
1:A:227:ASN:HD22	1:A:229:ASP:H	1.32	0.77
1:A:143:ASN:OD1	1:A:146:SER:HB2	1.82	0.77
1:A:163:ARG:CZ	2:A:280:NDP:H4B	2.20	0.72
2:A:280:NDP:O2A	2:A:280:NDP:P2B	2.48	0.72
1:A:1:ASP:OD2	1:A:51:HIS:HE1	1.75	0.70
1:A:163:ARG:NH1	2:A:280:NDP:H4B	2.07	0.69
1:A:219:GLN:O	1:A:220:ASN:CB	2.40	0.68
1:A:192:TRP:HE3	2:A:280:NDP:C5B	2.06	0.68
1:A:115:GLN:HE21	1:A:122:ARG:H	1.43	0.67
1:A:177:LYS:CG	1:A:178:THR:N	2.55	0.65
1:A:32:TYR:O	1:A:33:ASP:HB2	1.99	0.63
1:A:143:ASN:OD1	1:A:146:SER:CB	2.47	0.62
1:A:242:ASN:HD22	1:A:244:ASN:H	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LYS:HG2	1:A:178:THR:H	1.64	0.61
1:A:192:TRP:CB	2:A:280:NDP:O1A	2.48	0.59
1:A:192:TRP:HE3	2:A:280:NDP:H51A	1.68	0.58
1:A:193:SER:N	2:A:280:NDP:O1A	2.37	0.57
1:A:192:TRP:HE3	2:A:280:NDP:H52A	1.68	0.57
1:A:177:LYS:CG	1:A:178:THR:H	2.18	0.56
1:A:217:ASN:ND2	1:A:221:GLN:H	2.03	0.56
1:A:68:ASN:C	1:A:68:ASN:HD22	2.09	0.56
1:A:192:TRP:HB3	2:A:280:NDP:H51A	1.86	0.56
2:A:280:NDP:O2A	2:A:280:NDP:O2B	2.24	0.56
2:A:280:NDP:O1X	2:A:280:NDP:O2A	2.24	0.55
1:A:70:TYR:HA	2:A:280:NDP:C2A	2.36	0.54
2:A:280:NDP:O2D	2:A:280:NDP:C2N	2.55	0.54
1:A:160:GLU:OE1	2:A:280:NDP:H3B	2.10	0.51
1:A:163:ARG:NH1	2:A:280:NDP:C4B	2.73	0.51
1:A:227:ASN:HD22	1:A:229:ASP:N	2.06	0.49
1:A:192:TRP:CE3	2:A:280:NDP:C5B	2.92	0.49
1:A:51:HIS:HD2	1:A:61:SER:OG	1.96	0.48
1:A:166:PHE:H	1:A:236:ASN:ND2	2.12	0.48
1:A:160:GLU:OE2	2:A:280:NDP:H3B	2.14	0.47
1:A:115:GLN:HE21	1:A:122:ARG:N	2.13	0.47
1:A:192:TRP:CE3	2:A:280:NDP:H51A	2.48	0.46
1:A:192:TRP:CE3	2:A:280:NDP:H52A	2.50	0.46
1:A:192:TRP:N	2:A:280:NDP:O1A	2.48	0.46
1:A:1:ASP:OD2	1:A:51:HIS:CE1	2.64	0.45
1:A:177:LYS:HE2	1:A:178:THR:O	2.18	0.44
1:A:165:LYS:O	1:A:169:GLN:HG3	2.18	0.44
2:A:280:NDP:H8A	3:A:613:HOH:O	2.18	0.43
1:A:160:GLU:OE2	2:A:280:NDP:C2B	2.66	0.43
1:A:75:ARG:NH1	1:A:98:ASP:OD1	2.47	0.42
1:A:56:ALA:O	1:A:57:ASP:CB	2.66	0.42
1:A:192:TRP:CA	2:A:280:NDP:O1A	2.68	0.42
1:A:189:GLU:O	2:A:280:NDP:O2B	2.38	0.41
1:A:115:GLN:NE2	1:A:122:ARG:H	2.14	0.41
1:A:98:ASP:C	1:A:98:ASP:OD1	2.59	0.40
1:A:12:SER:O	1:A:16:VAL:HG13	2.22	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	245/247 (99%)	234 (96%)	10 (4%)	1 (0%)	39	20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	VAL

### 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	208/208 (100%)	187 (90%)	21 (10%)	9	2

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	27	ASN
1	A	28	GLU
1	A	29	ARG
1	A	33	ASP
1	A	57	ASP
1	A	68	ASN
1	A	69	VAL
1	A	78	ASP
1	A	84	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	101	ARG
1	A	107	TYR
1	A	173	LYS
1	A	180	LEU
1	A	186	ILE
1	A	217	ASN
1	A	219	GLN
1	A	227	ASN
1	A	236	ASN
1	A	242	ASN
1	A	246	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	45	GLN
1	A	51	HIS
1	A	68	ASN
1	A	84	ASN
1	A	115	GLN
1	A	145	ASN
1	A	156	GLN
1	A	170	GLN
1	A	217	ASN
1	A	227	ASN
1	A	236	ASN
1	A	242	ASN
1	A	244	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

1 ligand is 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	280	-	42,52,52	2.54	12 (28%)	55,80,80	3.27	25 (45%)

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	280	-	5/5/14/17	1/30/77/77	0/4/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	280	NDP	O2D-C2D	-7.49	1.25	1.43
2	A	280	NDP	O5B-C5B	-3.40	1.30	1.44
2	A	280	NDP	C5D-C4D	-3.00	1.41	1.51
2	A	280	NDP	O2B-C2B	-2.18	1.37	1.44
2	A	280	NDP	C5A-C4A	2.35	1.45	1.40
2	A	280	NDP	PA-O5B	2.87	1.72	1.59
2	A	280	NDP	C7N-N7N	3.31	1.42	1.33
2	A	280	NDP	C3B-C4B	3.99	1.63	1.53
2	A	280	NDP	O4D-C4D	4.51	1.55	1.45
2	A	280	NDP	O4B-C4B	4.56	1.55	1.45
2	A	280	NDP	C2A-N3A	5.08	1.41	1.32
2	A	280	NDP	O4B-C1B	7.12	1.50	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	280	NDP	C4B-O4B-C1B	-7.93	101.01	109.72
2	A	280	NDP	C1D-N1N-C2N	-7.19	108.38	120.91
2	A	280	NDP	O4B-C4B-C3B	-4.69	95.70	105.15
2	A	280	NDP	O4B-C1B-C2B	-4.39	98.66	106.60
2	A	280	NDP	C3B-C2B-C1B	-4.28	94.45	102.73
2	A	280	NDP	O4B-C1B-N9A	-3.82	100.11	108.10
2	A	280	NDP	O3-PA-O5B	-3.24	94.33	102.94
2	A	280	NDP	C6N-N1N-C2N	-2.42	112.28	118.52
2	A	280	NDP	O2N-PN-O5D	-2.07	98.05	108.46
2	A	280	NDP	O2D-C2D-C1D	2.08	117.21	109.94
2	A	280	NDP	O2D-C2D-C3D	2.19	118.95	111.83
2	A	280	NDP	O2N-PN-O1N	2.51	126.14	112.53
2	A	280	NDP	O3D-C3D-C2D	2.59	120.25	111.83
2	A	280	NDP	O2B-C2B-C1B	2.88	121.23	110.02
2	A	280	NDP	O7N-C7N-N7N	2.89	129.95	122.76
2	A	280	NDP	O5D-C5D-C4D	2.90	119.83	109.12
2	A	280	NDP	C3N-C2N-N1N	3.20	127.72	123.14
2	A	280	NDP	O2B-P2B-O1X	3.21	115.11	107.11
2	A	280	NDP	O3B-C3B-C4B	3.24	120.78	111.05
2	A	280	NDP	C2D-C3D-C4D	4.14	111.11	102.61
2	A	280	NDP	C1B-N9A-C4A	5.00	134.49	126.94
2	A	280	NDP	O3B-C3B-C2B	5.41	126.78	111.16
2	A	280	NDP	O4D-C1D-N1N	6.13	121.01	108.07
2	A	280	NDP	P2B-O2B-C2B	6.36	136.82	121.56
2	A	280	NDP	PN-O3-PA	10.53	162.29	132.73

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	280	NDP	C3D
2	A	280	NDP	C4B
2	A	280	NDP	C4D
2	A	280	NDP	C1B
2	A	280	NDP	C2D

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	280	NDP	P2B-O2B-C2B-C1B

There are no ring outliers.

1 monomer is involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	280	NDP	25	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 [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.