



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:05 AM UTC

PDB ID : 2GGS / pdb_00002ggs
Title : crystal structure of hypothetical dTDP-4-dehydrorhamnose reductase from
sulfolobus tokodaii
Authors : Rajakannan, V.; Mizushima, T.; Suzuki, A.; Masui, R.; Kuramitsu, S.; Ya-
mane, T.
Deposited on : 2006-03-24
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

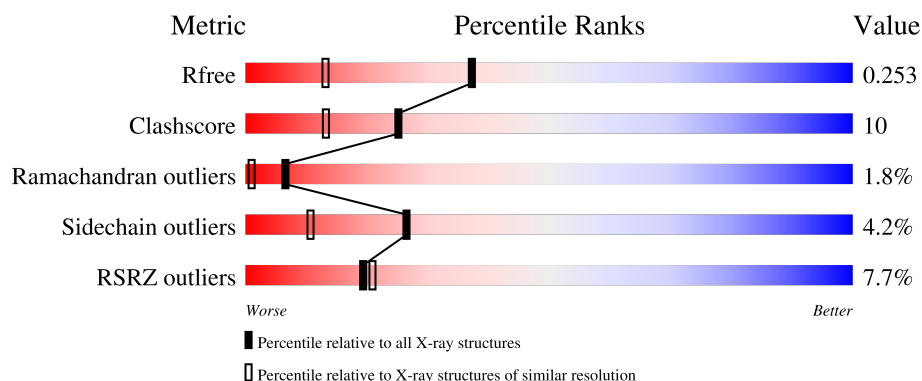
1 Overall quality at a glance

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))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	273	3% 86% 12% .
1	B	273	12% 79% 15% ..

2 Entry composition [i](#)

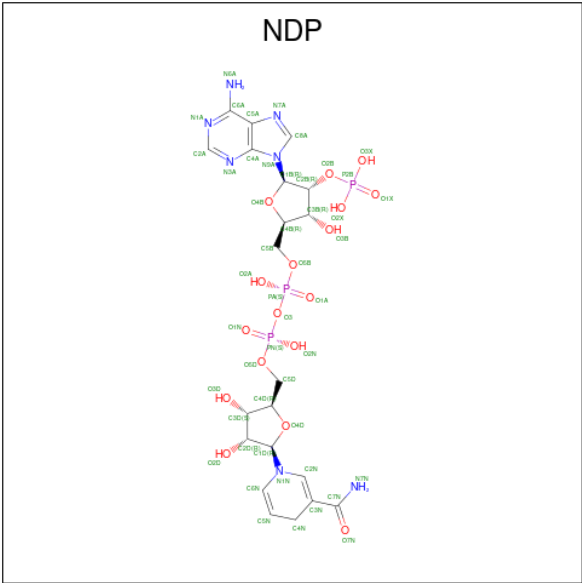
There are 3 unique types of molecules in this entry. The entry contains 4995 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 273aa long hypothetical dTDP-4-dehydrorhamnose reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2185	1402	369	410	4			
1	B	273	Total	C	N	O	S	0	0	0
			2184	1402	369	409	4			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

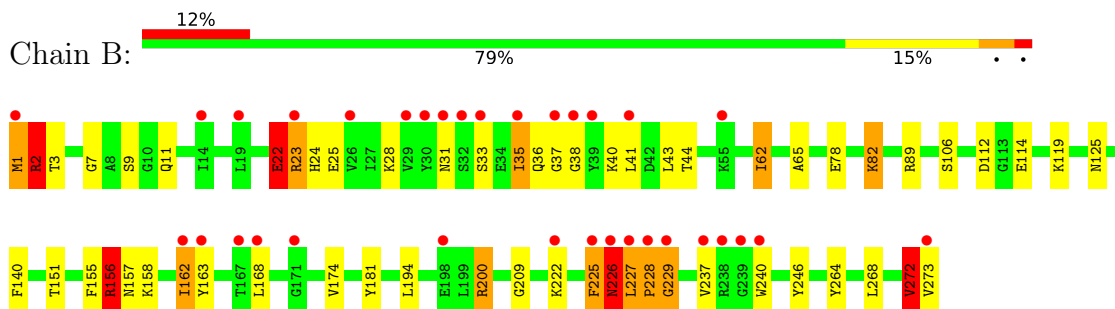
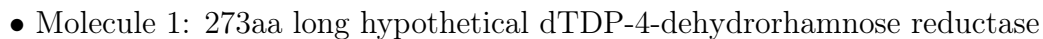


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	331	Total 331	O 331	0	0
3	B	199	Total 199	O 199	0	0

- Molecule 1: 273aa long hypothetical dTDP-4-dehydrorhamnose reductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.94Å 40.68Å 103.14Å 90.00° 116.18° 90.00°	Depositor
Resolution (Å)	19.87 – 1.70 19.87 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.87-1.70) 98.9 (19.87-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.20 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.253 0.206 , 0.253	Depositor DCC
R_{free} test set	3203 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4995	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.93	2/2223 (0.1%)	1.05	10/2991 (0.3%)
1	B	0.90	2/2222 (0.1%)	1.05	16/2991 (0.5%)
All	All	0.92	4/4445 (0.1%)	1.05	26/5982 (0.4%)

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
1	B	0	3
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	ILE	C-O	-8.86	1.14	1.24
1	B	272	VAL	C-O	-7.16	1.15	1.24
1	A	3	THR	C-O	-7.06	1.16	1.24
1	B	41	LEU	C-O	-6.36	1.16	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ARG	N-CA-C	10.42	128.61	114.12
1	B	226	ASN	N-CA-C	8.37	128.64	110.80
1	B	156	ARG	N-CA-C	8.21	123.12	112.12
1	A	3	THR	CA-C-N	7.96	133.04	122.30
1	A	3	THR	C-N-CA	7.96	133.04	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	TYR	N-CA-C	7.29	117.59	108.19
1	A	3	THR	O-C-N	-6.76	115.36	123.27
1	B	22	GLU	CA-C-N	6.70	133.75	121.70
1	B	22	GLU	C-N-CA	6.70	133.75	121.70
1	B	62	ILE	CB-CA-C	6.32	119.97	111.19
1	A	23	ARG	CA-C-N	6.09	133.17	121.54
1	A	23	ARG	C-N-CA	6.09	133.17	121.54
1	B	228	PRO	N-CA-C	5.99	124.82	112.47
1	A	181	TYR	N-CA-CB	-5.80	101.16	110.55
1	B	226	ASN	CA-C-N	5.77	132.09	121.70
1	B	226	ASN	C-N-CA	5.77	132.09	121.70
1	B	229	GLY	N-CA-C	-5.63	103.98	112.60
1	B	225	PHE	N-CA-C	5.46	119.44	112.12
1	B	229	GLY	CA-C-N	5.30	131.25	121.70
1	B	229	GLY	C-N-CA	5.30	131.25	121.70
1	B	2	ARG	N-CA-C	5.18	121.84	110.80
1	B	227	LEU	CA-C-N	5.09	126.20	119.84
1	B	227	LEU	C-N-CA	5.09	126.20	119.84
1	B	3	THR	N-CA-C	5.08	116.69	108.41
1	A	23	ARG	O-C-N	-5.01	116.46	122.27
1	A	4	LEU	O-C-N	5.00	128.89	123.13

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	TYR	Peptide
1	A	23	ARG	Peptide
1	A	272	VAL	Peptide
1	B	155	PHE	Peptide
1	B	225	PHE	Peptide
1	B	272	VAL	Peptide

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	2185	0	2243	31	0
1	B	2184	0	2243	53	0
2	A	48	0	26	3	0
2	B	48	0	26	11	0
3	A	331	0	0	6	0
3	B	199	0	0	4	0
All	All	4995	0	4538	87	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 10.

All (87) 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:B:22:GLU:CB	1:B:23:ARG:HB2	1.71	1.20
1:B:22:GLU:HB2	1:B:23:ARG:HB2	1.33	1.07
1:B:22:GLU:HB2	1:B:23:ARG:CB	1.86	1.05
1:B:7:GLY:HA2	2:B:901:NDP:H1B	1.39	1.05
1:A:200:ARG:HG2	1:A:200:ARG:HH11	1.22	1.00
1:B:200:ARG:HG2	1:B:200:ARG:HH11	1.28	0.96
1:B:22:GLU:HB3	1:B:23:ARG:HB2	1.49	0.91
1:A:20:LEU:O	1:A:24:HIS:HB2	1.75	0.86
1:A:200:ARG:HH11	1:A:200:ARG:CG	1.88	0.86
1:A:2:ARG:HD3	1:A:24:HIS:HD2	1.43	0.82
1:B:43:LEU:HB2	2:B:901:NDP:N1A	1.97	0.80
2:A:900:NDP:H41N	3:A:1134:HOH:O	1.85	0.76
1:B:7:GLY:CA	2:B:901:NDP:H1B	2.17	0.74
1:A:20:LEU:O	1:A:24:HIS:CB	2.35	0.74
1:B:200:ARG:HD2	3:B:1036:HOH:O	1.86	0.74
1:A:2:ARG:HD3	1:A:24:HIS:CD2	2.23	0.73
1:B:22:GLU:CB	1:B:23:ARG:CB	2.51	0.73
1:B:22:GLU:HB2	1:B:23:ARG:HB3	1.68	0.72
1:B:168:LEU:HB2	1:B:227:LEU:HD23	1.73	0.70
1:B:162:ILE:C	1:B:162:ILE:HD13	2.16	0.70
1:A:200:ARG:HG2	1:A:200:ARG:NH1	2.02	0.70
1:B:151:THR:O	2:B:901:NDP:H5N	1.92	0.69
1:B:1:MET:HA	1:B:1:MET:CE	2.24	0.68
1:B:226:ASN:H	1:B:227:LEU:HB2	1.58	0.68
1:B:1:MET:HA	1:B:1:MET:HE3	1.76	0.66
1:B:44:THR:HB	1:B:82:LYS:HG2	1.79	0.65
1:B:106:SER:O	2:B:901:NDP:H6N	1.95	0.65
1:B:1:MET:HE3	1:B:1:MET:CA	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:GLU:H	1:B:78:GLU:CD	2.06	0.64
1:B:200:ARG:HH11	1:B:200:ARG:CG	2.06	0.63
1:A:238:ARG:HG2	3:A:1014:HOH:O	1.97	0.62
1:A:1:MET:HG2	1:A:25:GLU:OE1	2.00	0.62
1:B:35:ILE:HG23	1:B:36:GLN:H	1.64	0.61
1:B:31:ASN:HB3	2:B:901:NDP:O3X	2.02	0.60
1:A:201:LYS:NZ	3:A:1052:HOH:O	2.35	0.59
2:A:900:NDP:C4N	3:A:1134:HOH:O	2.46	0.59
1:B:200:ARG:HG2	1:B:200:ARG:NH1	2.05	0.57
1:B:7:GLY:HA2	2:B:901:NDP:C1B	2.24	0.57
1:A:2:ARG:CD	1:A:24:HIS:HD2	2.16	0.56
1:B:36:GLN:HA	1:B:36:GLN:OE1	2.06	0.56
1:A:62:ILE:HD11	1:A:197:LEU:HD11	1.88	0.56
1:B:89:ARG:HD3	1:B:140:PHE:CE1	2.42	0.55
1:B:156:ARG:HG2	1:B:157:ASN:H	1.71	0.55
1:A:11:GLN:NE2	1:A:158:LYS:H	2.04	0.55
1:A:162:ILE:O	1:A:166:LYS:HG3	2.06	0.54
1:A:2:ARG:HB3	1:A:25:GLU:O	2.06	0.54
1:B:114:GLU:HG2	3:B:1021:HOH:O	2.09	0.53
1:A:268:LEU:HB3	1:A:271:MET:HE2	1.90	0.52
1:B:1:MET:HB3	1:B:25:GLU:OE1	2.10	0.51
1:B:157:ASN:HA	1:B:272:VAL:O	2.11	0.51
1:B:226:ASN:N	1:B:227:LEU:HB2	2.26	0.50
1:A:200:ARG:CG	1:A:200:ARG:NH1	2.57	0.49
1:B:112:ASP:HB3	1:B:125:ASN:O	2.13	0.49
1:A:20:LEU:O	1:A:24:HIS:HB3	2.14	0.48
1:B:2:ARG:CD	1:B:24:HIS:HD2	2.26	0.47
1:A:181:TYR:H	1:A:181:TYR:HD1	1.62	0.47
1:B:9:SER:OG	2:B:901:NDP:O1X	2.29	0.47
1:B:168:LEU:HD22	1:B:229:GLY:HA3	1.97	0.47
1:B:9:SER:HB3	1:B:33:SER:O	2.15	0.47
1:B:237:VAL:HB	1:B:240:TRP:CD2	2.50	0.47
1:A:222:LYS:NZ	1:A:227:LEU:O	2.48	0.47
1:A:273:VAL:HG22	3:A:1109:HOH:O	2.14	0.47
1:B:7:GLY:HA3	2:B:901:NDP:H4B	1.98	0.46
1:A:1:MET:HE3	1:A:1:MET:HB2	1.57	0.46
1:A:112:ASP:HB3	1:A:125:ASN:O	2.16	0.45
1:B:246:TYR:OH	3:B:1099:HOH:O	2.21	0.45
1:B:156:ARG:CG	1:B:157:ASN:N	2.80	0.45
1:B:11:GLN:NE2	1:B:158:LYS:H	2.15	0.45
1:B:163:TYR:HE2	1:B:174:VAL:HG13	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:TYR:CA	1:A:221:ILE:HD11	2.47	0.44
1:A:162:ILE:HG12	3:A:1126:HOH:O	2.19	0.43
1:B:1:MET:CE	1:B:1:MET:CA	2.91	0.43
1:A:106:SER:O	2:A:900:NDP:H6N	2.19	0.43
1:B:209:GLY:HA2	1:B:264:TYR:HA	2.01	0.43
1:A:1:MET:HG2	1:A:25:GLU:CD	2.44	0.42
1:B:168:LEU:CB	1:B:227:LEU:HD23	2.46	0.42
1:B:65:ALA:HA	2:B:901:NDP:O4B	2.19	0.42
1:B:168:LEU:HD13	1:B:222:LYS:HB2	2.02	0.42
1:B:36:GLN:O	1:B:38:GLY:N	2.53	0.41
1:B:156:ARG:HG2	1:B:157:ASN:N	2.35	0.41
1:A:1:MET:H3	1:A:25:GLU:HG2	1.85	0.41
1:A:195:GLU:HB3	1:A:259:LEU:HD22	2.03	0.41
1:A:258:ILE:HG22	1:A:259:LEU:HD23	2.01	0.41
1:A:139:THR:HA	1:A:142:LEU:HD12	2.02	0.41
1:B:28:LYS:O	1:B:38:GLY:HA2	2.21	0.41
2:B:901:NDP:H2N	2:B:901:NDP:H2D	1.72	0.40
1:B:200:ARG:CD	3:B:1036:HOH:O	2.58	0.40

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	271/273 (99%)	257 (95%)	12 (4%)	2 (1%)	18	7
1	B	271/273 (99%)	251 (93%)	12 (4%)	8 (3%)	3	0
All	All	542/546 (99%)	508 (94%)	24 (4%)	10 (2%)	6	1

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	B	2	ARG
1	B	23	ARG
1	B	37	GLY
1	B	22	GLU
1	B	226	ASN
1	B	228	PRO
1	A	156	ARG
1	B	35	ILE
1	B	272	VAL

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	237/237 (100%)	230 (97%)	7 (3%)	36	19
1	B	237/237 (100%)	224 (94%)	13 (6%)	19	6
All	All	474/474 (100%)	454 (96%)	20 (4%)	26	11

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

Mol	Chain	Res	Type
1	A	2	ARG
1	A	181	TYR
1	A	194	LEU
1	A	198	GLU
1	A	200	ARG
1	A	201	LYS
1	A	221	ILE
1	B	1	MET
1	B	2	ARG
1	B	40	LYS
1	B	62	ILE
1	B	82	LYS
1	B	119	LYS
1	B	156	ARG

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Mol	Chain	Res	Type
1	B	162	ILE
1	B	181	TYR
1	B	194	LEU
1	B	200	ARG
1	B	268	LEU
1	B	273	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	24	HIS
1	B	11	GLN
1	B	24	HIS
1	B	63	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 oligosaccharides 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	900	-	51,52,52	1.69	9 (17%)	71,80,80	1.64	14 (19%)
2	NDP	B	901	-	51,52,52	1.54	7 (13%)	71,80,80	1.77	12 (16%)

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	900	-	-	8/34/77/77	0/5/5/5
2	NDP	B	901	-	-	6/34/77/77	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	NDP	O7N-C7N	7.21	1.41	1.24
2	B	901	NDP	O7N-C7N	7.14	1.41	1.24
2	A	900	NDP	P2B-O2B	3.92	1.66	1.59
2	B	901	NDP	C2A-N1A	3.59	1.40	1.33
2	B	901	NDP	PA-O3	3.09	1.62	1.59
2	A	900	NDP	C2A-N1A	3.08	1.39	1.33
2	A	900	NDP	PA-O3	2.93	1.62	1.59
2	A	900	NDP	PN-O3	2.92	1.62	1.59
2	A	900	NDP	C8A-N7A	2.68	1.36	1.31
2	A	900	NDP	C6N-C5N	2.42	1.40	1.33
2	B	901	NDP	C2A-N3A	2.34	1.38	1.33
2	A	900	NDP	C5A-N7A	-2.32	1.34	1.39
2	B	901	NDP	C8A-N7A	2.30	1.36	1.31
2	B	901	NDP	C6N-C5N	2.24	1.39	1.33
2	A	900	NDP	C2A-N3A	2.21	1.37	1.33
2	B	901	NDP	P2B-O2B	2.03	1.63	1.59

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	NDP	N3A-C2A-N1A	-6.49	118.75	128.58
2	A	900	NDP	N3A-C2A-N1A	-6.49	118.76	128.58
2	B	901	NDP	C1D-N1N-C2N	-4.26	114.12	121.14
2	B	901	NDP	N9A-C8A-N7A	-4.25	107.91	113.94
2	B	901	NDP	C5A-C4A-N3A	-4.17	120.97	126.72
2	A	900	NDP	N9A-C8A-N7A	-4.00	108.26	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	NDP	C2A-N3A-C4A	3.82	121.16	111.83
2	B	901	NDP	C5A-N7A-C8A	3.65	109.19	103.45
2	B	901	NDP	O4B-C1B-N9A	3.59	114.98	108.09
2	B	901	NDP	N3A-C4A-N9A	3.32	132.81	127.17
2	A	900	NDP	C2A-N1A-C6A	3.10	123.83	118.73
2	A	900	NDP	C4A-N9A-C8A	3.04	108.94	105.74
2	A	900	NDP	O2A-PA-O3	3.04	115.50	107.27
2	A	900	NDP	C5A-N7A-C8A	2.74	107.75	103.45
2	A	900	NDP	C2A-N3A-C4A	2.73	118.50	111.83
2	A	900	NDP	C6N-N1N-C2N	2.62	122.12	119.32
2	A	900	NDP	O3-PA-O1A	-2.50	103.19	110.70
2	B	901	NDP	C4A-N9A-C8A	2.47	108.33	105.74
2	A	900	NDP	C5A-C4A-N3A	-2.44	123.35	126.72
2	A	900	NDP	O3D-C3D-C4D	-2.37	104.27	111.08
2	B	901	NDP	C2D-C1D-N1N	-2.31	107.63	113.31
2	A	900	NDP	O4B-C4B-C3B	2.26	109.64	105.15
2	B	901	NDP	P2B-O2B-C2B	-2.17	117.63	123.43
2	A	900	NDP	O2B-P2B-O1X	-2.14	101.71	109.33
2	B	901	NDP	O2A-PA-O3	2.11	112.97	107.27
2	A	900	NDP	C1D-N1N-C2N	-2.02	117.80	121.14

There are no chirality outliers.

All (14) torsion outliers are listed below:

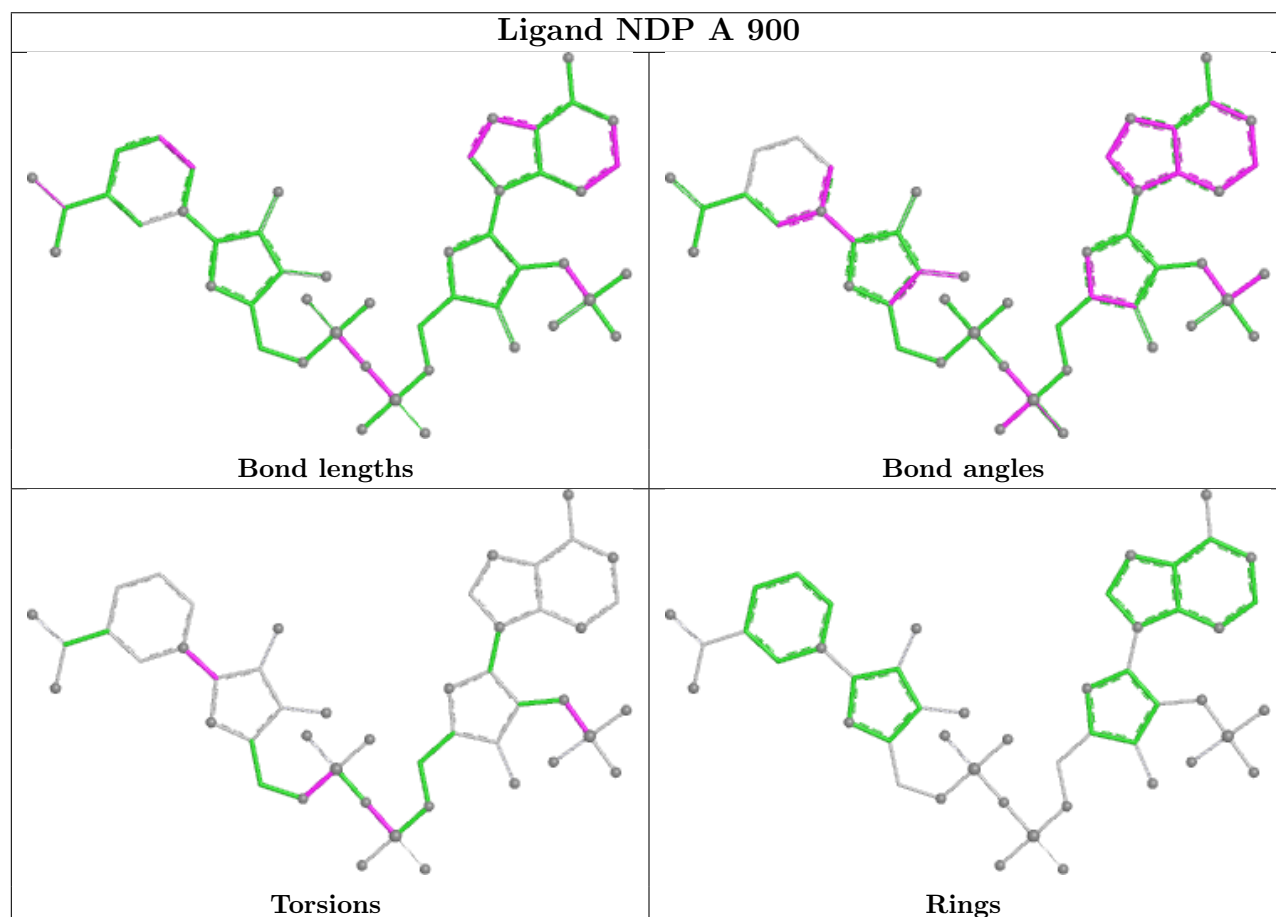
Mol	Chain	Res	Type	Atoms
2	A	900	NDP	C5D-O5D-PN-O3
2	A	900	NDP	C5D-O5D-PN-O1N
2	B	901	NDP	C5D-O5D-PN-O1N
2	B	901	NDP	C2D-C1D-N1N-C6N
2	A	900	NDP	PN-O3-PA-O1A
2	B	901	NDP	PN-O3-PA-O1A
2	A	900	NDP	C5D-O5D-PN-O2N
2	B	901	NDP	O4B-C4B-C5B-O5B
2	A	900	NDP	C2B-O2B-P2B-O3X
2	A	900	NDP	O4D-C1D-N1N-C6N
2	B	901	NDP	O4D-C1D-N1N-C6N
2	A	900	NDP	C2D-C1D-N1N-C6N
2	A	900	NDP	PN-O3-PA-O2A
2	B	901	NDP	PN-O3-PA-O2A

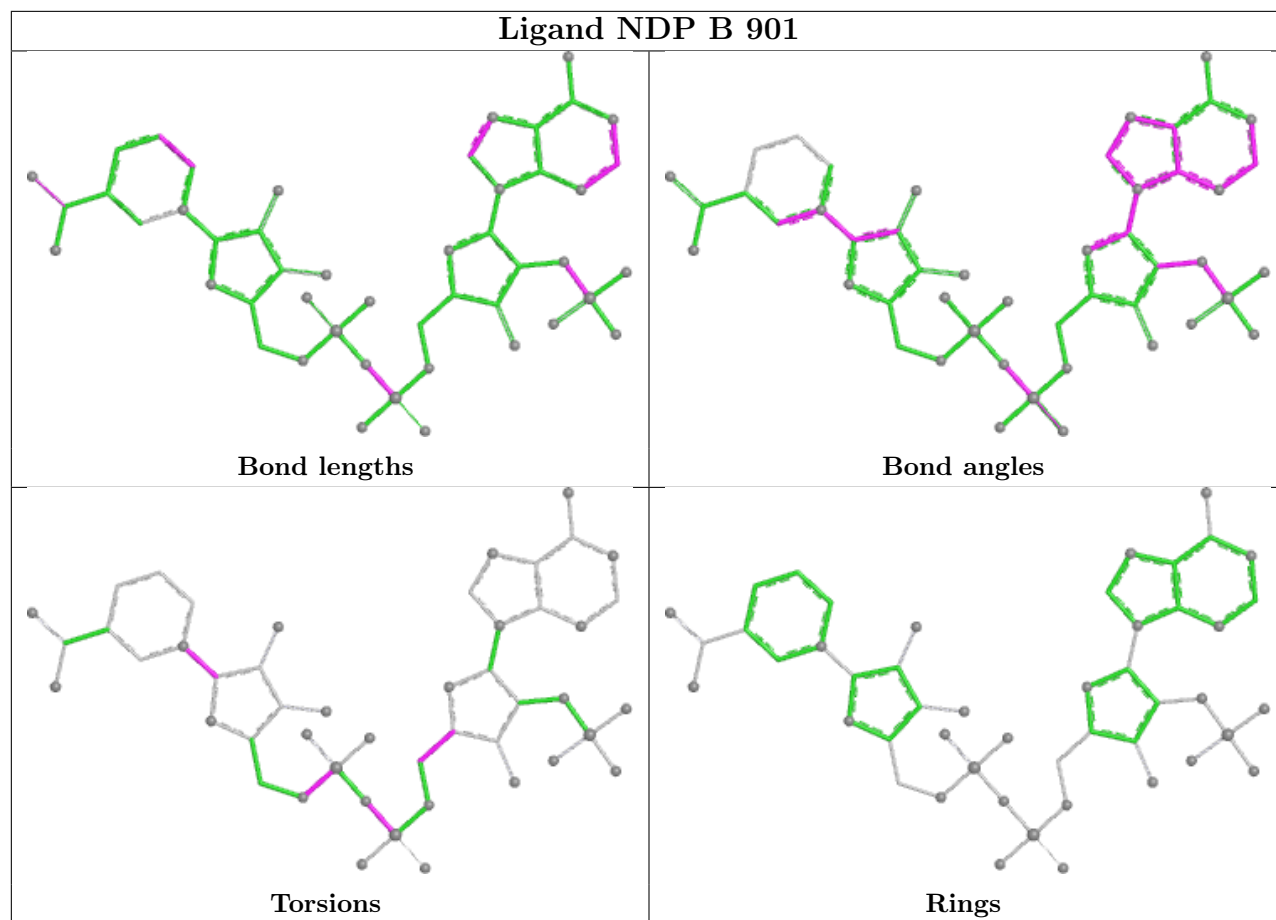
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	NDP	3	0
2	B	901	NDP	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 95th 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	273/273 (100%)	0.02	9 (3%) 49 53	12, 21, 34, 43	0
1	B	273/273 (100%)	0.72	33 (12%) 8 8	14, 29, 51, 61	0
All	All	546/546 (100%)	0.37	42 (7%) 19 21	12, 24, 46, 61	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	LEU	6.4
1	B	226	ASN	6.1
1	B	273	VAL	5.2
1	B	37	GLY	4.7
1	B	1	MET	4.5
1	B	229	GLY	4.2
1	A	1	MET	4.0
1	B	38	GLY	3.8
1	B	39	TYR	3.7
1	A	273	VAL	3.5
1	B	32	SER	3.5
1	B	237	VAL	3.3
1	A	170	GLU	3.2
1	B	239	GLY	3.0
1	B	35	ILE	2.9
1	B	238	ARG	2.8
1	B	225	PHE	2.7
1	B	222	LYS	2.7
1	B	26	VAL	2.7
1	B	23	ARG	2.6
1	B	228	PRO	2.6
1	B	55	LYS	2.6
1	B	33	SER	2.6
1	A	20	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	30	TYR	2.5
1	B	41	LEU	2.5
1	B	168	LEU	2.5
1	B	31	ASN	2.4
1	B	19	LEU	2.4
1	A	198	GLU	2.3
1	A	261	THR	2.3
1	B	240	TRP	2.3
1	B	29	VAL	2.3
1	B	171	GLY	2.3
1	B	163	TYR	2.2
1	B	167	THR	2.2
1	B	14	ILE	2.2
1	A	236	GLU	2.1
1	B	198	GLU	2.1
1	B	162	ILE	2.1
1	A	75	ILE	2.1
1	A	24	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95th 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.

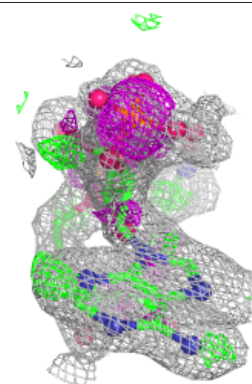
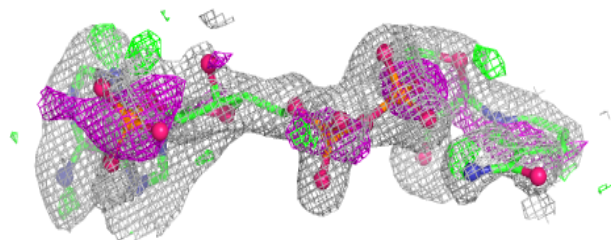
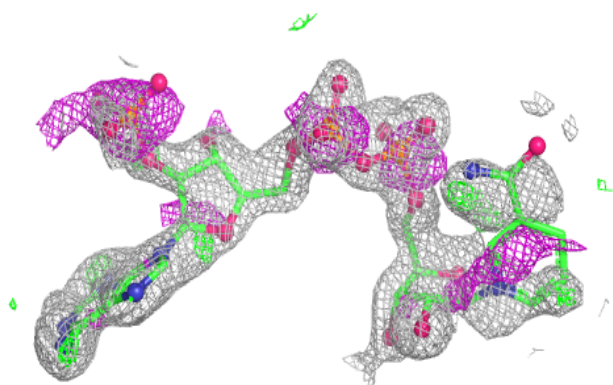
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NDP	B	901	48/48	0.79	0.15	22,36,49,52	0
2	NDP	A	900	48/48	0.97	0.07	13,16,33,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

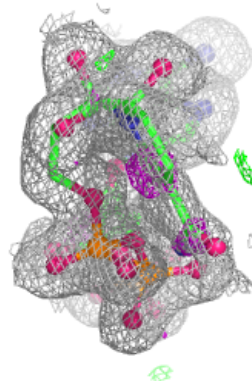
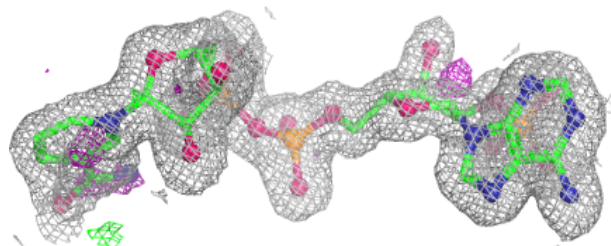
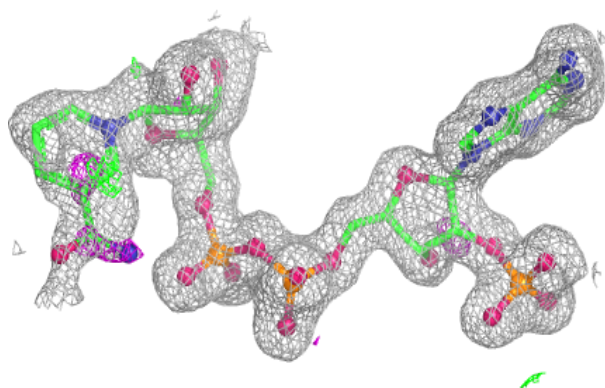
Electron density around NDP B 901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NDP A 900:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.