



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 01:55 PM EDT

PDB ID : 3MJV  
Title : Structure of A-type Ketoreductases from Modular Polyketide Synthase  
Authors : Zheng, J.; Taylor, C.A.; Piasecki, S.K.; Keatinge-Clay, A.T.  
Deposited on : 2010-04-13  
Resolution : 1.46 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

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

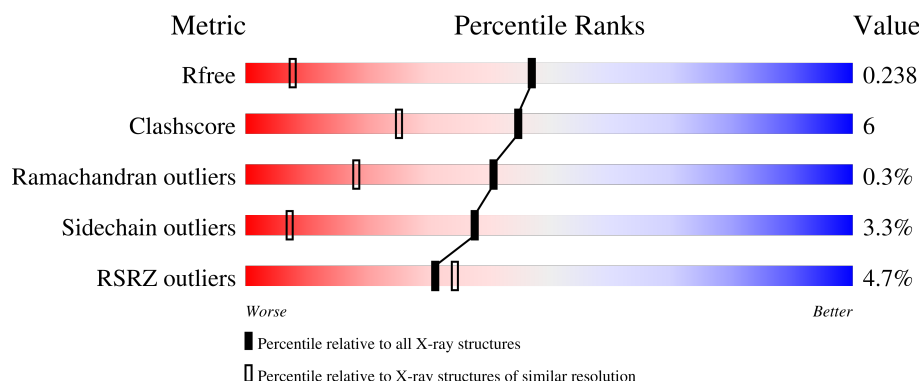
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.46 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))
$R_{free}$	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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  $\geq 3$ , 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	496	<div> <div>4%</div> <div>79%</div> <div>15%</div> <div>..</div> </div>
1	B	496	<div> <div>5%</div> <div>80%</div> <div>14%</div> <div>..</div> </div>

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	476	X	-	-	-
2	NDP	B	476	X	-	-	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7547 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 AmphB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3462	2161	634	658	9			
1	B	475	Total	C	N	O	S	0	0	0
			3456	2158	633	656	9			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q93NW7
A	-19	GLY	-	expression tag	UNP Q93NW7
A	-18	SER	-	expression tag	UNP Q93NW7
A	-17	SER	-	expression tag	UNP Q93NW7
A	-16	HIS	-	expression tag	UNP Q93NW7
A	-15	HIS	-	expression tag	UNP Q93NW7
A	-14	HIS	-	expression tag	UNP Q93NW7
A	-13	HIS	-	expression tag	UNP Q93NW7
A	-12	HIS	-	expression tag	UNP Q93NW7
A	-11	HIS	-	expression tag	UNP Q93NW7
A	-10	SER	-	expression tag	UNP Q93NW7
A	-9	SER	-	expression tag	UNP Q93NW7
A	-8	GLY	-	expression tag	UNP Q93NW7
A	-7	LEU	-	expression tag	UNP Q93NW7
A	-6	VAL	-	expression tag	UNP Q93NW7
A	-5	PRO	-	expression tag	UNP Q93NW7
A	-4	ARG	-	expression tag	UNP Q93NW7
A	-3	GLY	-	expression tag	UNP Q93NW7
A	-2	SER	-	expression tag	UNP Q93NW7
A	-1	HIS	-	expression tag	UNP Q93NW7
A	0	MET	-	expression tag	UNP Q93NW7
A	359	PHE	TRP	engineered mutation	UNP Q93NW7
B	-20	MET	-	expression tag	UNP Q93NW7
B	-19	GLY	-	expression tag	UNP Q93NW7
B	-18	SER	-	expression tag	UNP Q93NW7

*Continued on next page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP Q93NW7
B	-16	HIS	-	expression tag	UNP Q93NW7
B	-15	HIS	-	expression tag	UNP Q93NW7
B	-14	HIS	-	expression tag	UNP Q93NW7
B	-13	HIS	-	expression tag	UNP Q93NW7
B	-12	HIS	-	expression tag	UNP Q93NW7
B	-11	HIS	-	expression tag	UNP Q93NW7
B	-10	SER	-	expression tag	UNP Q93NW7
B	-9	SER	-	expression tag	UNP Q93NW7
B	-8	GLY	-	expression tag	UNP Q93NW7
B	-7	LEU	-	expression tag	UNP Q93NW7
B	-6	VAL	-	expression tag	UNP Q93NW7
B	-5	PRO	-	expression tag	UNP Q93NW7
B	-4	ARG	-	expression tag	UNP Q93NW7
B	-3	GLY	-	expression tag	UNP Q93NW7
B	-2	SER	-	expression tag	UNP Q93NW7
B	-1	HIS	-	expression tag	UNP Q93NW7
B	0	MET	-	expression tag	UNP Q93NW7
B	359	PHE	TRP	engineered mutation	UNP Q93NW7

- 
- The chemical structure of NDP (Nucleoside Diphosphate) is shown. It consists of a ribose sugar (C1-C5) linked to a pyrimidine nucleobase (C6-C9) via a glycosidic bond. The sugar has hydroxyl groups at C2' and C3', and a phosphate group at C5'. The phosphate group is linked to a pyrophosphate chain (P1, P2) which is further linked to a third phosphate group (P3). The nucleobase has an amino group at C4 and a carbonyl group at C6. The structure is labeled with various atoms and bonds, including C1, C2, C3, C4, C5, C6, C7, C8, C9, N1, N2, N3, N4, N5, N6, N7, N8, N9, O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100, O101, O102, O103, O104, O105, O106, O107, O108, O109, O110, O111, O112, O113, O114, O115, O116, O117, O118, O119, O120, O121, O122, O123, O124, O125, O126, O127, O128, O129, O130, O131, O132, O133, O134, O135, O136, O137, O138, O139, O140, O141, O142, O143, O144, O145, O146, O147, O148, O149, O150, O151, O152, O153, O154, O155, O156, O157, O158, O159, O160, O161, O162, O163, O164, O165, O166, O167, O168, O169, O170, O171, O172, O173, O174, O175, O176, O177, O178, O179, O180, O181, O182, O183, O184, O185, O186, O187, O188, O189, O190, O191, O192, O193, O194, O195, O196, O197, O198, O199, O200, O201, O202, O203, O204, O205, O206, O207, O208, O209, O210, O211, O212, O213, O214, O215, O216, O217, O218, O219, O220, O221, O222, O223, O224, O225, O226, O227, O228, O229, O230, O231, O232, O233, O234, O235, O236, O237, O238, O239, O240, O241, O242, O243, O244, O245, O246, O247, O248, O249, O250, O251, O252, O253, O254, O255, O256, O257, O258, O259, O260, O261, O262, O263, O264, O265, O266, O267, O268, O269, O270, O271, O272, O273, O274, O275, O276, O277, O278, O279, O280, O281, O282, O283, O284, O285, O286, O287, O288, O289, O290, O291, O292, O293, O294, O295, O296, O297, O298, O299, O300, O301, O302, O303, O304, O305, O306, O307, O308, O309, O310, O311, O312, O313, O314, O315, O316, O317, O318, O319, O320, O321, O322, O323, O324, O325, O326, O327, O328, O329, O330, O331, O332, O333, O334, O335, O336, O337, O338, O339, O340, O341, O342, O343, O344, O345, O346, O347, O348, O349, O350, O351, O352, O353, O354, O355, O356, O357, O358, O359, O360, O361, O362, O363, O364, O365, O366, O367, O368, O369, O370, O371, O372, O373, O374, O375, O376, O377, O378, O379, O380, O381, O382, O383, O384, O385, O386, O387, O388, O389, O390, O391, O392, O393, O394, O395, O396, O397, O398, O399, O400, O401, O402, O403, O404, O405, O406, O407, O408, O409, O410, O411, O412, O413, O414, O415, O416, O417, O418, O419, O420, O421, O422, O423, O424, O425, O426, O427, O428, O429, O430, O431, O432, O433, O434, O435, O436, O437, O438, O439, O440, O441, O442, O443, O444, O445, O446, O447, O448, O449, O450, O451, O452, O453, O454, O455, O456, O457, O458, O459, O460, O461, O462, O463, O464, O465, O466, O467, O468, O469, O470, O471, O472, O473, O474, O475, O476, O477, O478, O479, O480, O481, O482, O483, O484, O485, O486, O487, O488, O489, O490, O491, O492, O493, O494, O495, O496, O497, O498, O499, O500, O501, O502, O503, O504, O505, O506, O507, O508, O509, O510, O511, O512, O513, O514, O515, O516, O517, O518, O519, O520, O521, O522, O523, O524, O525, O526, O527, O528, O529, O530, O531, O532, O533, O534, O535, O536, O537, O538, O539, O540, O541, O542, O543, O544, O545, O546, O547, O548, O549, O550, O551, O552, O553, O554, O555, O556, O557, O558, O559, O560, O561, O562, O563, O564, O565, O566, O567, O568, O569, O570, O571, O572, O573, O574, O575, O576, O577, O578, O579, O580, O581, O582, O583, O584, O585, O586, O587, O588, O589, O590, O591, O592, O593, O594, O595, O596, O597, O598, O599, O600, O601, O602, O603, O604, O605, O606, O607, O608, O609, O610, O611, O612, O613, O614, O615, O616, O617, O618, O619, O620, O621, O622, O623, O624, O625, O626, O627, O628, O629, O630, O631, O632, O633, O634, O635, O636, O637, O638, O639, O640, O641, O642, O643, O644, O645, O646, O647, O648, O649, O650, O651, O652, O653, O654, O655, O656, O657, O658, O659, O660, O661, O662, O663, O664, O665, O666, O667, O668, O669, O670, O671, O672, O673, O674, O675, O676, O677, O678, O679, O680, O681, O682, O683, O684, O685, O686, O687, O688, O689, O690, O691, O692, O693, O694, O695, O696, O697, O698, O699, O700, O701, O702, O703, O704, O705, O706, O707, O708, O709, O710, O711, O712, O713, O714, O715, O716, O717, O718, O719, O720, O721, O722, O723, O724, O725, O726, O727, O728, O729, O730, O731, O732, O733, O734, O735, O736, O737, O738, O739, O740, O741, O742, O743, O744, O745, O746, O747, O748, O749, O750, O751, O752, O753, O754, O755, O756, O757, O758, O759, O760, O761, O762, O763, O764, O765, O766, O767, O768, O769, O770, O771, O772, O773, O774, O775, O776, O777, O778, O779, O780, O781, O782, O783, O784, O785, O786, O787, O788, O789, O790, O791, O792, O793, O794, O795, O796

*Continued on next page...*

*Continued from previous page...*

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

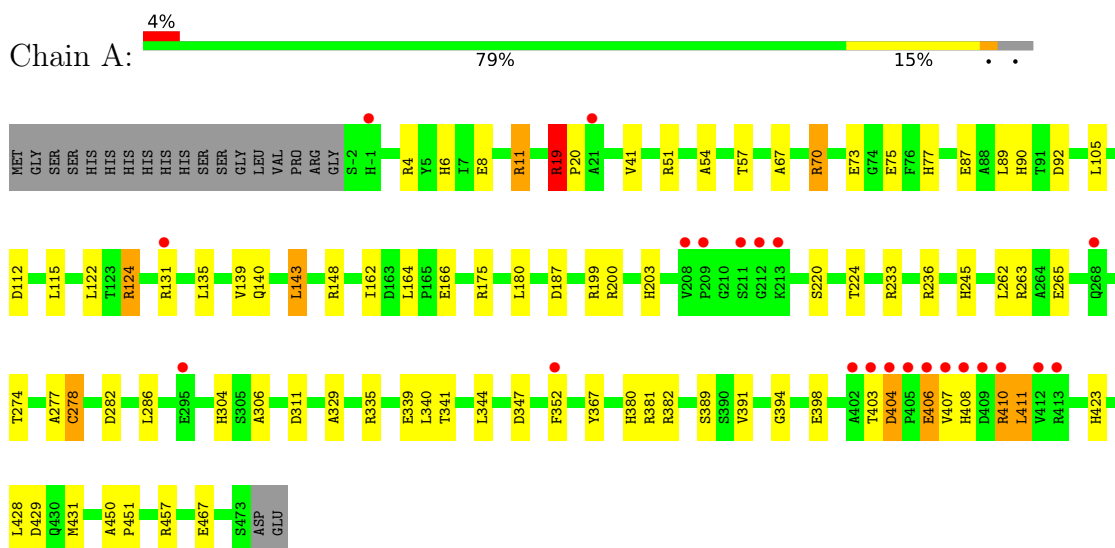
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	254	Total	O	0	0
			254	254		
3	B	279	Total	O	0	0
			279	279		

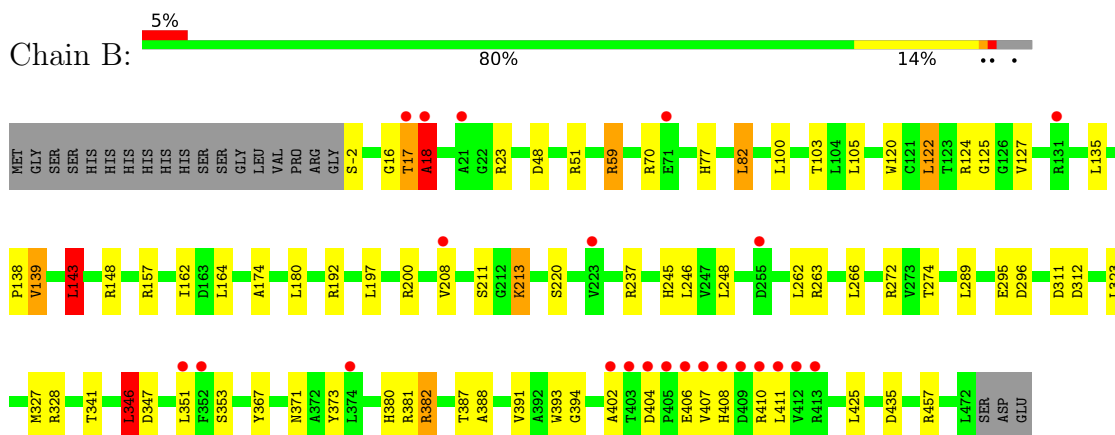
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: AmphB



#### • Molecule 1: AmphB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.50Å 63.69Å 71.92Å 72.93° 67.21° 89.76°	Depositor
Resolution (Å)	50.00 – 1.46 26.60 – 1.46	Depositor EDS
% Data completeness (in resolution range)	82.9 (50.00-1.46) 82.9 (26.60-1.46)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.199 , 0.236 0.200 , 0.238	Depositor DCC
$R_{free}$ test set	6885 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.115 for h,-k,h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7547	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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	1.26	9/3531 (0.3%)	1.24	28/4822 (0.6%)
1	B	1.26	9/3525 (0.3%)	1.35	39/4814 (0.8%)
All	All	1.26	18/7056 (0.3%)	1.29	67/9636 (0.7%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	TRP	CG-CD1	6.71	1.46	1.36
1	A	367	TYR	CD1-CE1	6.42	1.49	1.39
1	B	295	GLU	CB-CG	6.16	1.63	1.52
1	A	457	ARG	CB-CG	-6.07	1.36	1.52
1	A	389	SER	CA-CB	6.03	1.61	1.52
1	B	367	TYR	CG-CD1	6.01	1.47	1.39
1	A	278	CYS	CB-SG	-5.96	1.72	1.81
1	B	18	ALA	CA-CB	-5.83	1.40	1.52
1	A	381	ARG	CB-CG	-5.78	1.36	1.52
1	A	73	GLU	CB-CG	5.58	1.62	1.52
1	B	295	GLU	CG-CD	5.49	1.60	1.51
1	B	127	VAL	CB-CG2	5.47	1.64	1.52
1	B	127	VAL	CB-CG1	5.36	1.64	1.52
1	B	139	VAL	CB-CG2	-5.26	1.41	1.52
1	B	457	ARG	CB-CG	-5.19	1.38	1.52
1	A	54	ALA	CA-CB	5.09	1.63	1.52
1	A	339	GLU	CB-CG	5.04	1.61	1.52
1	A	352	PHE	CE2-CZ	5.04	1.47	1.37

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	ARG	NE-CZ-NH1	24.44	132.52	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	ARG	NE-CZ-NH2	-20.34	110.13	120.30
1	A	381	ARG	NE-CZ-NH2	-10.55	115.03	120.30
1	B	148	ARG	NE-CZ-NH2	-10.23	115.18	120.30
1	A	381	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	A	200	ARG	NE-CZ-NH2	-9.91	115.34	120.30
1	B	51	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	B	382	ARG	CD-NE-CZ	9.46	136.85	123.60
1	A	4	ARG	NE-CZ-NH2	-9.01	115.80	120.30
1	B	122	LEU	CB-CG-CD2	8.92	126.17	111.00
1	B	200	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	A	51	ARG	NE-CZ-NH1	-8.72	115.94	120.30
1	B	382	ARG	CB-CG-CD	8.59	133.94	111.60
1	B	82	LEU	CB-CG-CD1	8.38	125.25	111.00
1	B	148	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	19	ARG	NE-CZ-NH2	8.20	124.40	120.30
1	B	157	ARG	NE-CZ-NH1	-8.13	116.24	120.30
1	B	51	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	A	143	LEU	CB-CG-CD2	-8.03	97.36	111.00
1	A	19	ARG	NE-CZ-NH1	-7.95	116.32	120.30
1	B	263	ARG	NE-CZ-NH1	-7.61	116.49	120.30
1	A	200	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	B	381	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	B	391	VAL	CA-CB-CG2	7.06	121.48	110.90
1	B	263	ARG	NE-CZ-NH2	6.97	123.79	120.30
1	B	272	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	A	382	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	B	391	VAL	CG1-CB-CG2	6.62	121.50	110.90
1	B	59	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	B	164	LEU	CA-CB-CG	-6.40	100.58	115.30
1	B	328	ARG	NE-CZ-NH1	-6.39	117.10	120.30
1	B	391	VAL	CB-CA-C	-6.37	99.30	111.40
1	B	200	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	192	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	187	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	429	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	B	346	LEU	CB-CG-CD2	6.09	121.36	111.00
1	B	70	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	A	278	CYS	CA-CB-SG	-5.97	103.25	114.00
1	A	347	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	A	4	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	367	TYR	CG-CD1-CE1	-5.79	116.67	121.30
1	A	367	TYR	CB-CG-CD2	-5.77	117.54	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	192	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	164	LEU	CB-CG-CD1	5.75	120.77	111.00
1	A	263	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	B	312	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	105	LEU	CB-CG-CD2	-5.55	101.56	111.00
1	B	289	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	A	175	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	311	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	199	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	410	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	410	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	B	347	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	197	LEU	CB-CG-CD1	-5.32	101.95	111.00
1	B	143	LEU	CB-CG-CD2	5.31	120.03	111.00
1	B	296	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	282	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	70	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	B	59	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	B	381	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	148	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	246	LEU	CB-CG-CD1	-5.09	102.35	111.00
1	A	112	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	B	346	LEU	CB-CG-CD1	5.00	119.50	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3462	0	3425	48	0
1	B	3456	0	3420	42	0
2	A	48	0	25	1	0
2	B	48	0	25	2	0
3	A	254	0	0	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	279	0	0	6	0
All	All	7547	0	6895	90	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 6.

All (90) 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:16:GLY:O	1:B:17:THR:O	1.62	1.17
1:B:262:LEU:O	1:B:266:LEU:HD13	1.49	1.11
1:B:17:THR:HG23	1:B:174:ALA:HB1	1.16	1.08
1:A:90:HIS:HD2	1:A:92:ASP:H	1.14	0.90
1:A:236:ARG:HB3	3:A:532:HOH:O	1.74	0.86
1:B:17:THR:CG2	1:B:174:ALA:HB1	2.03	0.83
1:B:59:ARG:HB2	1:B:105:LEU:CD1	2.16	0.76
1:B:17:THR:O	1:B:18:ALA:HB2	1.86	0.76
1:B:16:GLY:O	1:B:17:THR:C	2.25	0.76
1:A:306:ALA:N	3:A:530:HOH:O	2.20	0.74
1:A:391:VAL:HG21	1:A:428:LEU:HD13	1.70	0.73
1:B:404:ASP:O	1:B:408:HIS:HB3	1.89	0.72
1:B:208:VAL:HG23	1:B:211:SER:OG	1.88	0.72
1:A:90:HIS:CD2	1:A:92:ASP:H	2.04	0.71
1:A:341:THR:HA	1:A:344:LEU:HD13	1.71	0.71
1:A:203:HIS:HD2	3:A:533:HOH:O	1.73	0.71
1:A:245:HIS:HE1	1:A:274:THR:OG1	1.73	0.71
1:B:237:ARG:HD2	1:B:425:LEU:HD13	1.74	0.70
1:A:203:HIS:HE1	1:A:467:GLU:OE2	1.75	0.69
1:A:404:ASP:O	1:A:408:HIS:HB3	1.93	0.69
1:A:404:ASP:OD2	1:A:406:GLU:HB2	1.93	0.67
1:A:11:ARG:CZ	1:A:11:ARG:HB2	2.24	0.66
1:B:103:THR:HG21	1:B:143:LEU:HD11	1.78	0.66
1:B:245:HIS:HE1	1:B:274:THR:OG1	1.78	0.65
1:B:262:LEU:C	1:B:262:LEU:HD23	2.20	0.62
1:A:277:ALA:O	1:A:278:CYS:HB3	2.00	0.61
1:B:402:ALA:O	1:B:408:HIS:HB2	2.01	0.61
1:A:166:GLU:H	1:A:166:GLU:CD	2.06	0.59
1:B:213:LYS:HD2	1:B:435:ASP:HB2	1.87	0.57
1:B:18:ALA:HB3	3:B:637:HOH:O	2.05	0.57
1:A:124:ARG:H	1:A:140:GLN:NE2	2.03	0.56
1:A:394:GLY:O	2:A:476:NDP:H42N	2.06	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLU:OE2	1:A:139:VAL:CG2	2.54	0.55
1:B:59:ARG:HB2	1:B:105:LEU:HD12	1.89	0.55
1:B:135:LEU:O	1:B:380:HIS:HD2	1.89	0.55
1:A:67:ALA:O	1:A:70:ARG:HG3	2.06	0.55
1:A:77:HIS:HE1	1:A:180:LEU:O	1.89	0.55
1:A:41:VAL:HG21	1:A:164:LEU:HD11	1.90	0.54
1:A:135:LEU:O	1:A:380:HIS:HD2	1.89	0.54
1:B:393:TRP:HB2	2:B:476:NDP:C5N	2.37	0.54
1:A:6:HIS:NE2	1:A:8:GLU:OE1	2.40	0.54
1:B:17:THR:O	1:B:18:ALA:CB	2.56	0.54
1:A:87:GLU:OE2	1:A:139:VAL:HG21	2.07	0.53
1:B:341:THR:HB	1:B:346:LEU:HD22	1.91	0.53
1:A:391:VAL:HG21	1:A:428:LEU:CD1	2.37	0.52
1:A:57:THR:OG1	1:A:90:HIS:HE1	1.93	0.51
1:B:139:VAL:HG22	3:B:550:HOH:O	2.09	0.51
1:B:248:LEU:HD11	1:B:262:LEU:HD21	1.94	0.50
1:B:77:HIS:HE1	1:B:180:LEU:O	1.94	0.49
1:B:237:ARG:CD	1:B:425:LEU:HD13	2.40	0.49
1:A:304:HIS:HE1	1:A:329:ALA:O	1.95	0.49
1:B:351:LEU:CD2	3:B:529:HOH:O	2.60	0.48
1:B:351:LEU:HD23	3:B:529:HOH:O	2.14	0.48
1:A:220:SER:OG	1:A:245:HIS:HD2	1.97	0.48
1:A:304:HIS:CD2	3:A:530:HOH:O	2.66	0.47
1:A:410:ARG:HG3	1:A:411:LEU:N	2.29	0.47
1:A:304:HIS:CE1	1:A:329:ALA:O	2.68	0.47
1:A:41:VAL:CG2	1:A:164:LEU:HD11	2.44	0.47
1:B:220:SER:OG	1:B:245:HIS:HD2	1.98	0.47
1:A:233:ARG:HD2	1:A:236:ARG:HD3	1.96	0.47
1:B:404:ASP:O	1:B:408:HIS:CB	2.61	0.47
1:B:387:THR:HG22	3:B:705:HOH:O	2.15	0.46
1:A:19:ARG:HB2	1:A:20:PRO:HD2	1.97	0.46
1:A:139:VAL:HG22	3:A:581:HOH:O	2.14	0.46
1:A:224:THR:OG1	1:A:304:HIS:HD2	1.97	0.46
1:A:245:HIS:CE1	1:A:274:THR:OG1	2.62	0.46
1:B:125:GLY:HA2	3:B:600:HOH:O	2.16	0.46
1:A:404:ASP:O	1:A:408:HIS:CB	2.62	0.46
1:A:89:LEU:HD11	1:A:335:ARG:HH22	1.80	0.45
1:A:224:THR:OG1	1:A:304:HIS:CD2	2.69	0.45
1:B:382:ARG:HD3	1:B:388:ALA:O	2.17	0.45
1:A:124:ARG:H	1:A:140:GLN:HE22	1.64	0.44
1:A:391:VAL:HG22	1:A:431:MET:SD	2.57	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLU:C	1:A:403:THR:HG21	2.37	0.44
1:A:122:LEU:HD22	1:A:162:ILE:HB	2.00	0.43
1:B:122:LEU:HD22	1:B:162:ILE:HB	1.99	0.43
1:A:286:LEU:HD23	1:A:340:LEU:HD12	2.00	0.43
1:A:406:GLU:HB3	1:A:407:VAL:H	1.48	0.42
1:B:394:GLY:O	2:B:476:NDP:H42N	2.19	0.42
1:B:341:THR:HB	1:B:346:LEU:CD2	2.50	0.42
1:B:353:SER:HA	1:B:371:ASN:OD1	2.19	0.42
1:A:19:ARG:HB2	1:A:19:ARG:HE	1.39	0.42
1:B:100:LEU:HA	1:B:143:LEU:HD22	2.01	0.42
1:B:262:LEU:O	1:B:262:LEU:HD23	2.20	0.41
1:A:115:LEU:N	1:A:115:LEU:HD12	2.36	0.41
1:B:138:PRO:HB2	1:B:373:TYR:CE1	2.56	0.41
1:B:407:VAL:O	1:B:411:LEU:HD12	2.20	0.41
1:A:450:ALA:HB3	1:A:451:PRO:HD3	2.02	0.41
1:B:323:LEU:O	1:B:327:MET:HG2	2.21	0.41
1:B:135:LEU:O	1:B:380:HIS:CD2	2.73	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	474/496 (96%)	458 (97%)	15 (3%)	1 (0%)	47	22
1	B	473/496 (95%)	462 (98%)	9 (2%)	2 (0%)	34	13
All	All	947/992 (96%)	920 (97%)	24 (2%)	3 (0%)	41	18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLU

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	17	THR
1	B	18	ALA

### 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	334/351 (95%)	322 (96%)	12 (4%)	35	6
1	B	333/351 (95%)	323 (97%)	10 (3%)	41	9
All	All	667/702 (95%)	645 (97%)	22 (3%)	38	7

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	19	ARG
1	A	75	GLU
1	A	124	ARG
1	A	131	ARG
1	A	143	LEU
1	A	262	LEU
1	A	265	GLU
1	A	311	ASP
1	A	404	ASP
1	A	411	LEU
1	A	423	HIS
1	B	-2	SER
1	B	23	ARG
1	B	48	ASP
1	B	82	LEU
1	B	124	ARG
1	B	143	LEU
1	B	213	LYS
1	B	346	LEU
1	B	406	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	410	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	77	HIS
1	A	90	HIS
1	A	102	GLN
1	A	140	GLN
1	A	203	HIS
1	A	245	HIS
1	A	304	HIS
1	A	336	HIS
1	A	380	HIS
1	B	32	HIS
1	B	77	HIS
1	B	102	GLN
1	B	245	HIS
1	B	336	HIS
1	B	380	HIS

### 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 monosaccharides 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	B	476	-	45,52,52	1.44	6 (13%)	53,80,80	2.26	14 (26%)
2	NDP	A	476	-	45,52,52	1.52	7 (15%)	53,80,80	1.96	10 (18%)

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	B	476	-	1/1/14/17	8/30/77/77	0/5/5/5
2	NDP	A	476	-	1/1/14/17	7/30/77/77	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	476	NDP	C4N-C3N	-4.43	1.41	1.49
2	B	476	NDP	C4A-N3A	4.16	1.41	1.35
2	A	476	NDP	P2B-O2B	3.75	1.66	1.59
2	A	476	NDP	C6N-C5N	3.46	1.39	1.33
2	B	476	NDP	C4N-C5N	-3.06	1.40	1.48
2	A	476	NDP	C4N-C5N	-3.03	1.41	1.48
2	B	476	NDP	P2B-O2B	3.01	1.65	1.59
2	B	476	NDP	C4N-C3N	-2.93	1.44	1.49
2	B	476	NDP	O7N-C7N	-2.83	1.17	1.24
2	B	476	NDP	C6N-C5N	2.42	1.37	1.33
2	A	476	NDP	O4D-C1D	2.40	1.47	1.42
2	A	476	NDP	C6N-N1N	-2.18	1.31	1.37
2	A	476	NDP	C1D-N1N	2.05	1.52	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	476	NDP	C2B-C3B-C4B	-7.38	85.97	101.99

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	476	NDP	C2B-C3B-C4B	-6.93	86.93	101.99
2	B	476	NDP	N3A-C2A-N1A	-6.29	118.84	128.68
2	A	476	NDP	O4B-C4B-C3B	5.55	116.09	105.11
2	B	476	NDP	C2A-N1A-C6A	5.05	127.39	118.75
2	A	476	NDP	N3A-C2A-N1A	-4.80	121.18	128.68
2	B	476	NDP	O4B-C4B-C3B	4.50	114.01	105.11
2	B	476	NDP	C5B-C4B-C3B	3.61	128.71	115.18
2	B	476	NDP	C1B-N9A-C4A	-3.59	120.34	126.64
2	B	476	NDP	O7N-C7N-C3N	-3.43	114.43	120.90
2	B	476	NDP	O2B-P2B-O1X	-3.36	96.41	109.39
2	A	476	NDP	O3B-C3B-C4B	3.08	119.96	111.05
2	A	476	NDP	C5B-C4B-C3B	2.94	126.21	115.18
2	B	476	NDP	O4B-C1B-C2B	-2.92	101.52	106.59
2	B	476	NDP	O3B-C3B-C4B	2.84	119.26	111.05
2	A	476	NDP	C2A-N1A-C6A	2.81	123.56	118.75
2	B	476	NDP	C3N-C7N-N7N	2.80	122.64	117.67
2	B	476	NDP	C1D-N1N-C6N	-2.65	115.12	120.83
2	A	476	NDP	C1B-N9A-C4A	-2.65	121.99	126.64
2	A	476	NDP	O4B-C4B-C5B	2.53	117.69	109.37
2	A	476	NDP	O2B-P2B-O1X	-2.50	99.75	109.39
2	B	476	NDP	O3X-P2B-O2X	2.29	116.40	107.64
2	B	476	NDP	O2A-PA-O1A	2.17	122.99	112.24
2	A	476	NDP	O4B-C1B-C2B	-2.07	102.99	106.59

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	476	NDP	C4B
2	B	476	NDP	C4B

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	476	NDP	O4B-C4B-C5B-O5B
2	A	476	NDP	C5D-O5D-PN-O2N
2	B	476	NDP	O4B-C4B-C5B-O5B
2	B	476	NDP	C5D-O5D-PN-O1N
2	B	476	NDP	C5D-O5D-PN-O2N
2	B	476	NDP	C3B-C4B-C5B-O5B
2	A	476	NDP	O4D-C1D-N1N-C6N
2	B	476	NDP	O4D-C1D-N1N-C6N
2	A	476	NDP	C3B-C4B-C5B-O5B

*Continued on next page...*

*Continued from previous page...*

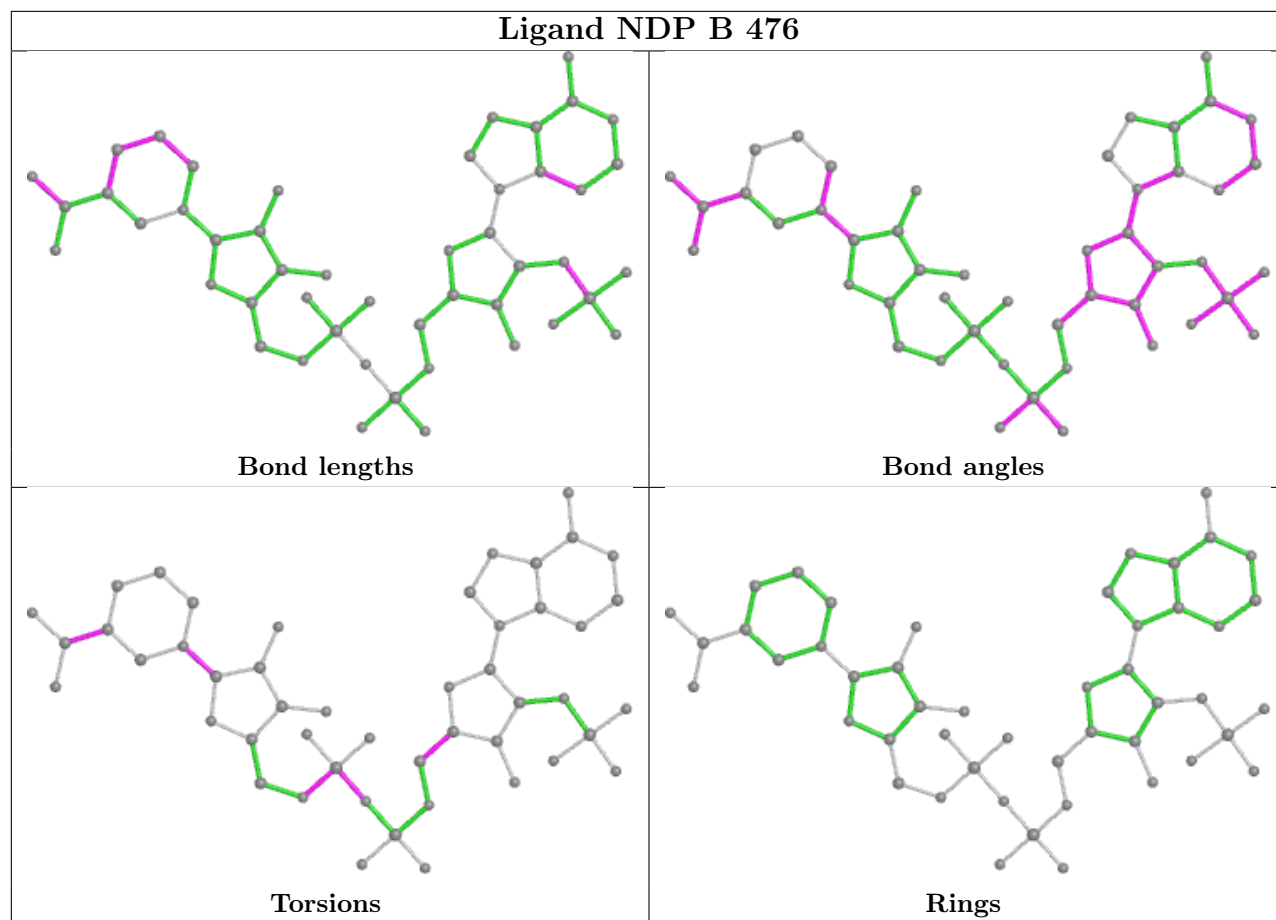
Mol	Chain	Res	Type	Atoms
2	A	476	NDP	C5D-O5D-PN-O3
2	A	476	NDP	C5D-O5D-PN-O1N
2	B	476	NDP	PA-O3-PN-O2N
2	B	476	NDP	C5D-O5D-PN-O3
2	A	476	NDP	PA-O3-PN-O2N
2	B	476	NDP	C2N-C3N-C7N-N7N

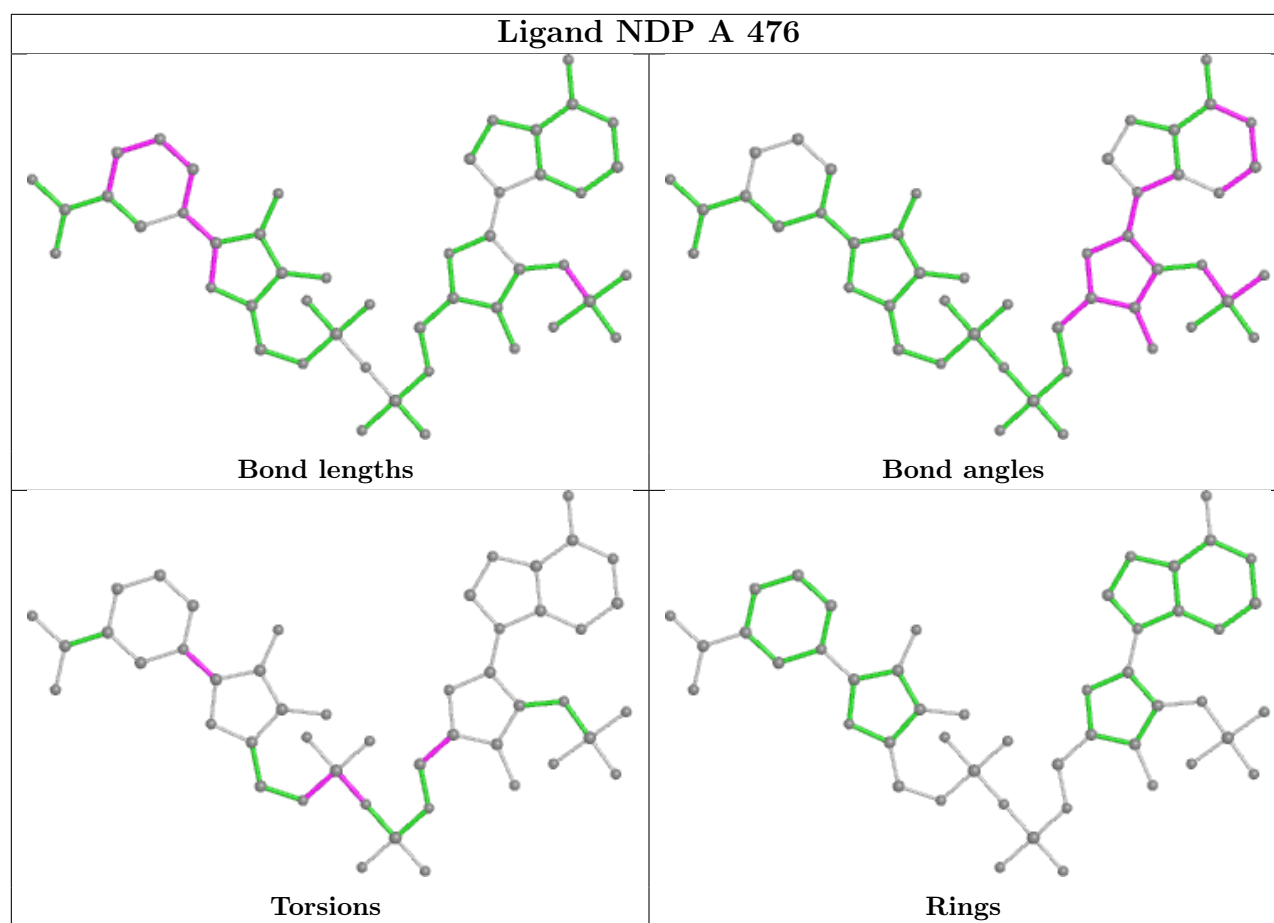
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	476	NDP	2	0
2	A	476	NDP	1	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, 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	476/496 (95%)	0.13	22 (4%) 32 35	9, 16, 32, 67	0
1	B	475/496 (95%)	0.13	23 (4%) 30 33	8, 15, 30, 64	0
All	All	951/992 (95%)	0.13	45 (4%) 31 34	8, 16, 32, 67	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	VAL	7.5
1	B	405	PRO	6.6
1	A	402	ALA	6.3
1	A	405	PRO	5.9
1	A	404	ASP	5.2
1	A	403	THR	4.8
1	B	17	THR	4.2
1	A	406	GLU	4.2
1	B	131	ARG	3.9
1	A	408	HIS	3.8
1	B	411	LEU	3.7
1	B	18	ALA	3.6
1	A	131	ARG	3.5
1	A	413	ARG	3.4
1	B	408	HIS	3.4
1	A	213	LYS	3.3
1	A	410	ARG	3.2
1	B	406	GLU	3.2
1	B	407	VAL	3.2
1	A	208	VAL	3.1
1	A	409	ASP	3.0
1	B	409	ASP	3.0
1	A	412	VAL	3.0
1	B	413	ARG	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	403	THR	2.7
1	A	352	PHE	2.7
1	B	412	VAL	2.7
1	B	352	PHE	2.6
1	A	212	GLY	2.5
1	A	209	PRO	2.4
1	A	295	GLU	2.3
1	B	404	ASP	2.3
1	B	71	GLU	2.3
1	B	351	LEU	2.3
1	B	21	ALA	2.2
1	B	402	ALA	2.2
1	A	211	SER	2.2
1	B	208	VAL	2.2
1	B	374	LEU	2.2
1	A	268	GLN	2.2
1	B	410	ARG	2.1
1	A	-1	HIS	2.1
1	A	21	ALA	2.1
1	B	223	VAL	2.1
1	B	255	ASP	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](#)

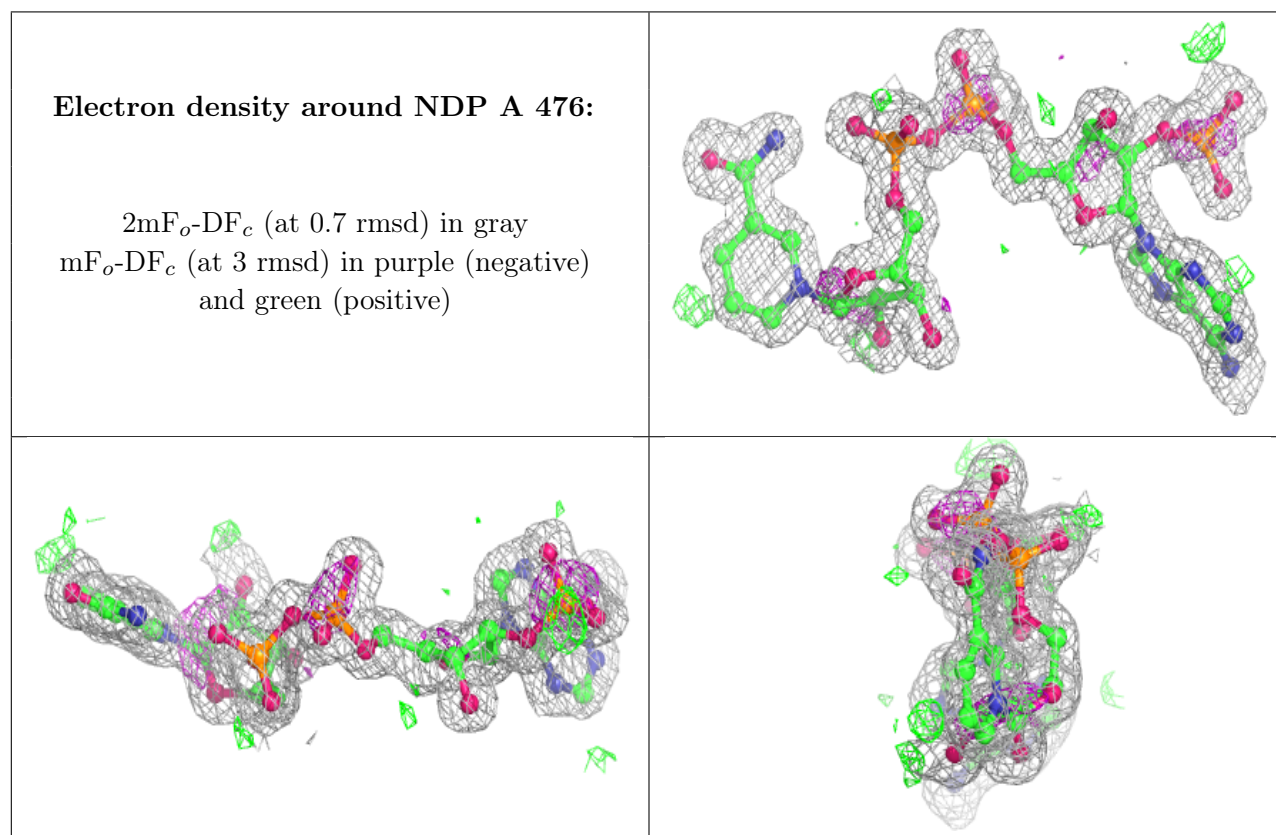
There are no monosaccharides in this entry.

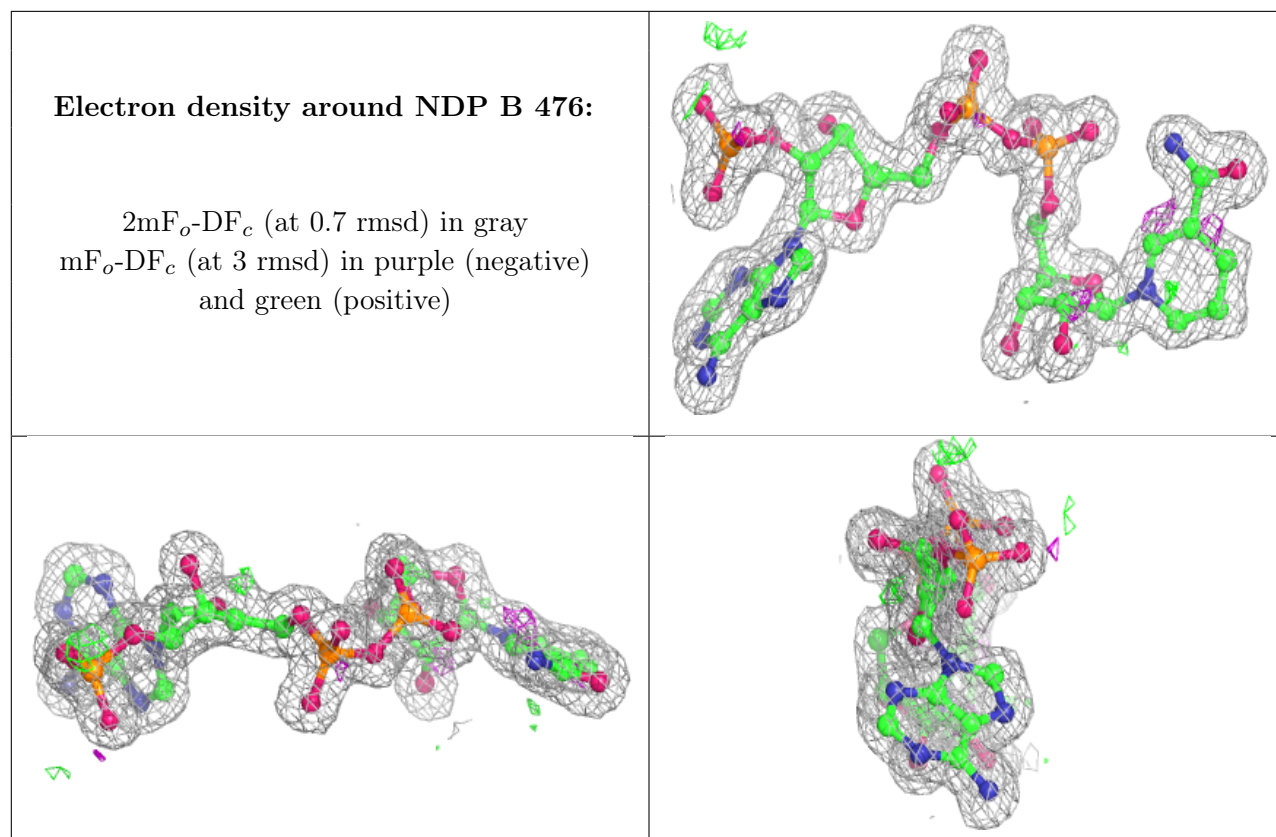
## 6.4 Ligands [i](#)

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, 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NDP	A	476	48/48	0.96	0.11	16,21,25,25	0
2	NDP	B	476	48/48	0.98	0.07	12,17,20,22	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.