



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:59 pm BST

PDB ID : 3MJE
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 : 2010-04-12
Resolution : 1.36 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 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 : 2.11
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) : 2.11

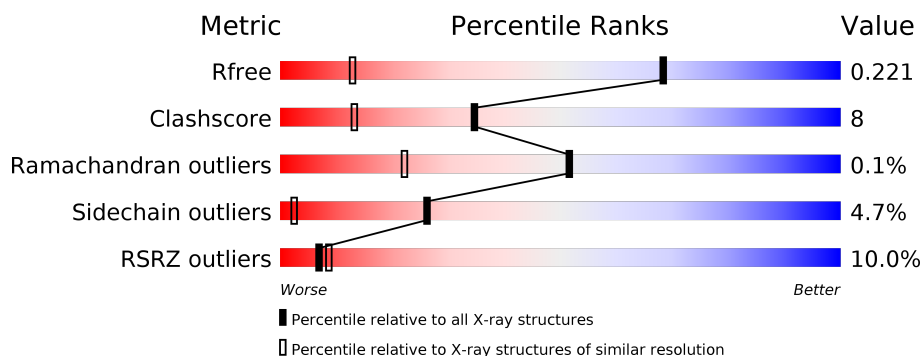
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.36 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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 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>10%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>•• 5%</div> </div> </div>
1	B	496	<div> <div>9%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>•• 6%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7404 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	470	Total	C	N	O	S	0	0	0
			3422	2137	629	647	9			
1	B	468	Total	C	N	O	S	0	0	0
			3406	2128	625	644	9			

There are 42 discrepancies between the modelled and reference sequences:

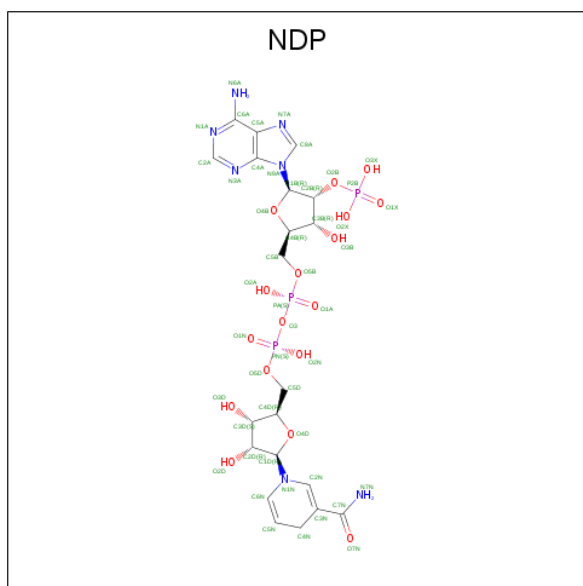
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q93NW7
A	-19	GLY	-	EXPRESSION TAG	UNP Q93NW7
A	-18	SER	-	EXPRESSION TAG	UNP Q93NW7
A	-17	SER	-	EXPRESSION TAG	UNP Q93NW7
A	-16	HIS	-	EXPRESSION TAG	UNP Q93NW7
A	-15	HIS	-	EXPRESSION TAG	UNP Q93NW7
A	-14	HIS	-	EXPRESSION TAG	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
B	-20	MET	-	EXPRESSION TAG	UNP Q93NW7
B	-19	GLY	-	EXPRESSION TAG	UNP Q93NW7
B	-18	SER	-	EXPRESSION TAG	UNP Q93NW7
B	-17	SER	-	EXPRESSION TAG	UNP Q93NW7

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- 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 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

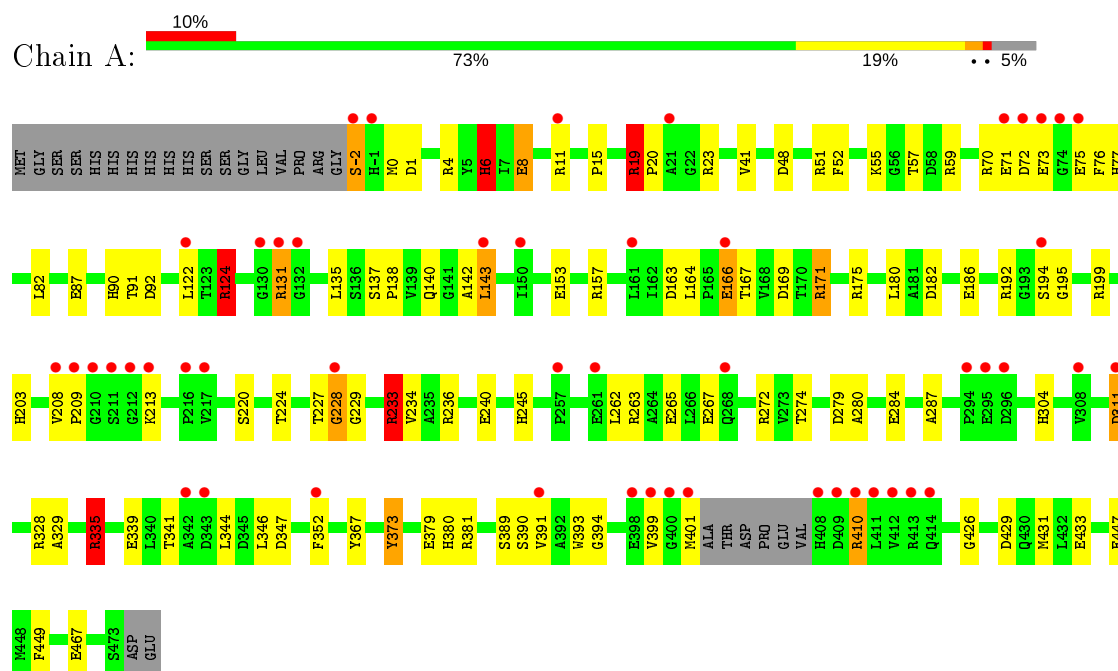
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	227	Total	O	0	0
			227	227		
4	B	247	Total	O	0	0
			247	247		

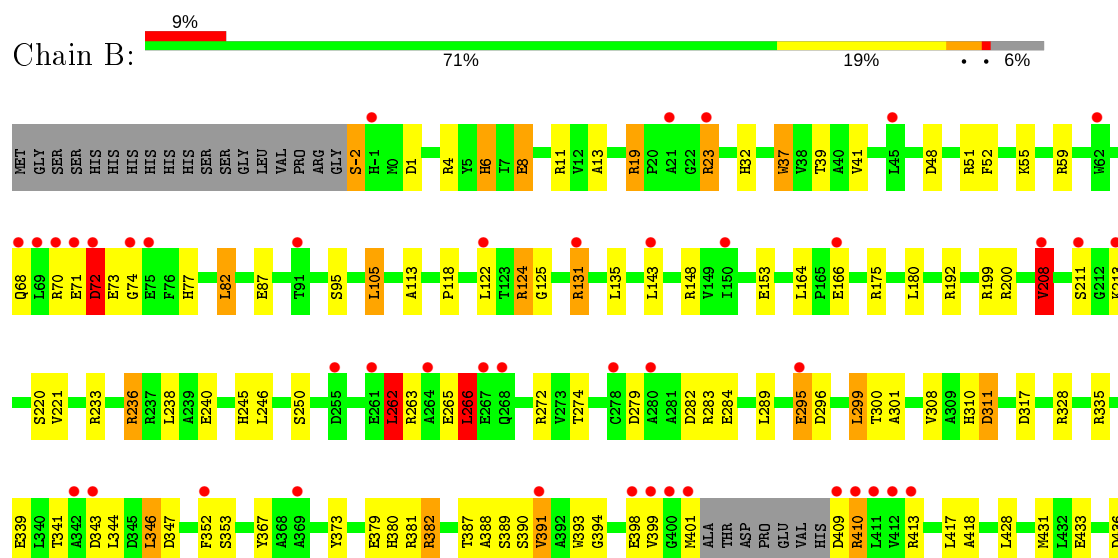
3 Residue-property plots [i](#)

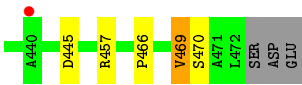
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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, α , β , γ	61.65Å 63.76Å 71.74Å 72.99° 67.21° 89.79°	Depositor
Resolution (Å)	62.76 – 1.36 31.38 – 1.36	Depositor EDS
% Data completeness (in resolution range)	93.3 (62.76-1.36) 93.3 (31.38-1.36)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 1.36Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.202 , 0.225 0.200 , 0.221	Depositor DCC
R_{free} test set	9658 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.059 for h,-k,h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7404	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: GOL, 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	1.58	42/3490 (1.2%)	1.55	49/4764 (1.0%)
1	B	1.55	36/3473 (1.0%)	1.57	70/4741 (1.5%)
All	All	1.56	78/6963 (1.1%)	1.56	119/9505 (1.3%)

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	1
All	All	0	4

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	GLU	CB-CG	-15.02	1.23	1.52
1	A	166	GLU	CG-CD	-13.15	1.32	1.51
1	B	469	VAL	CB-CG2	-10.96	1.29	1.52
1	B	284	GLU	CB-CG	-10.91	1.31	1.52
1	A	389	SER	CA-CB	-10.57	1.37	1.52
1	B	379	GLU	CD-OE1	-10.19	1.14	1.25
1	A	284	GLU	CB-CG	-9.37	1.34	1.52
1	A	389	SER	CB-OG	-9.07	1.30	1.42
1	B	166	GLU	C-O	8.68	1.39	1.23
1	B	39	THR	CB-CG2	-8.26	1.25	1.52
1	B	105	LEU	CG-CD1	-8.00	1.22	1.51
1	B	39	THR	CB-OG1	-7.84	1.27	1.43
1	A	390	SER	CB-OG	-7.82	1.32	1.42
1	B	52	PHE	CG-CD1	-7.78	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	LYS	CB-CG	-7.77	1.31	1.52
1	B	166	GLU	CG-CD	-7.77	1.40	1.51
1	B	390	SER	CB-OG	-7.64	1.32	1.42
1	B	87	GLU	CD-OE2	-7.44	1.17	1.25
1	A	433	GLU	CG-CD	7.43	1.63	1.51
1	B	-2	SER	CB-OG	7.42	1.51	1.42
1	A	52	PHE	CG-CD2	-7.42	1.27	1.38
1	B	284	GLU	CD-OE1	-7.15	1.17	1.25
1	A	381	ARG	CB-CG	-7.00	1.33	1.52
1	A	284	GLU	CD-OE2	-6.97	1.18	1.25
1	A	367	TYR	CD1-CE1	6.87	1.49	1.39
1	A	15	PRO	CG-CD	6.82	1.73	1.50
1	A	8	GLU	CD-OE2	-6.79	1.18	1.25
1	A	71	GLU	CG-CD	-6.68	1.42	1.51
1	B	166	GLU	CD-OE1	-6.67	1.18	1.25
1	B	95	SER	CB-OG	6.47	1.50	1.42
1	B	113	ALA	CA-CB	6.45	1.66	1.52
1	A	-2	SER	CB-OG	6.44	1.50	1.42
1	B	284	GLU	CG-CD	-6.43	1.42	1.51
1	A	19	ARG	CZ-NH1	-6.41	1.24	1.33
1	B	124	ARG	NE-CZ	6.38	1.41	1.33
1	A	87	GLU	CD-OE1	-6.33	1.18	1.25
1	B	399	VAL	CB-CG1	-6.31	1.39	1.52
1	A	335	ARG	CB-CG	-6.29	1.35	1.52
1	A	91	THR	CB-CG2	-6.27	1.31	1.52
1	A	6	HIS	CA-CB	-6.12	1.40	1.53
1	A	166	GLU	CD-OE1	-6.11	1.19	1.25
1	B	143	LEU	CG-CD1	-5.99	1.29	1.51
1	A	228	GLY	C-O	-5.96	1.14	1.23
1	A	137	SER	CB-OG	5.94	1.50	1.42
1	A	76	PHE	CE2-CZ	-5.91	1.26	1.37
1	B	398	GLU	CD-OE1	-5.83	1.19	1.25
1	B	272	ARG	CZ-NH2	-5.65	1.25	1.33
1	A	367	TYR	CE2-CZ	-5.64	1.31	1.38
1	A	153	GLU	CG-CD	-5.64	1.43	1.51
1	B	389	SER	CB-OG	5.63	1.49	1.42
1	B	124	ARG	CZ-NH2	-5.63	1.25	1.33
1	B	317	ASP	CG-OD2	-5.61	1.12	1.25
1	A	73	GLU	CB-CG	5.59	1.62	1.52
1	B	457	ARG	CB-CG	-5.58	1.37	1.52
1	A	328	ARG	CZ-NH2	-5.54	1.25	1.33
1	A	379	GLU	CD-OE1	-5.51	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	399	VAL	CB-CG2	-5.50	1.41	1.52
1	A	143	LEU	CG-CD2	-5.46	1.31	1.51
1	B	250	SER	CB-OG	5.46	1.49	1.42
1	A	52	PHE	CD2-CE2	5.44	1.50	1.39
1	A	410	ARG	CZ-NH1	5.41	1.40	1.33
1	B	262	LEU	CG-CD2	-5.40	1.31	1.51
1	A	234	VAL	CB-CG2	-5.39	1.41	1.52
1	B	8	GLU	CD-OE2	-5.37	1.19	1.25
1	A	142	ALA	CA-CB	5.36	1.63	1.52
1	A	449	PHE	CD1-CE1	5.36	1.50	1.39
1	B	433	GLU	CB-CG	5.35	1.62	1.52
1	B	391	VAL	CB-CG2	5.33	1.64	1.52
1	A	124	ARG	CG-CD	-5.32	1.38	1.51
1	A	399	VAL	CB-CG2	-5.30	1.41	1.52
1	A	272	ARG	CZ-NH1	-5.26	1.26	1.33
1	A	287	ALA	CA-CB	5.24	1.63	1.52
1	B	295	GLU	CG-CD	-5.24	1.44	1.51
1	A	240	GLU	CD-OE2	-5.19	1.20	1.25
1	A	186	GLU	CD-OE2	-5.17	1.20	1.25
1	A	267	GLU	CB-CG	5.16	1.61	1.52
1	B	208	VAL	CB-CG2	-5.11	1.42	1.52
1	B	418	ALA	CA-CB	5.07	1.63	1.52

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	ARG	NE-CZ-NH2	-21.13	109.74	120.30
1	B	382	ARG	NE-CZ-NH1	20.25	130.43	120.30
1	A	328	ARG	NE-CZ-NH2	-19.54	110.53	120.30
1	B	382	ARG	CD-NE-CZ	17.09	147.53	123.60
1	A	19	ARG	NE-CZ-NH2	15.42	128.01	120.30
1	A	55	LYS	CD-CE-NZ	-14.82	77.61	111.70
1	A	328	ARG	NE-CZ-NH1	14.77	127.69	120.30
1	A	311	ASP	CB-CG-OD1	13.92	130.83	118.30
1	A	175	ARG	NE-CZ-NH2	-13.45	113.57	120.30
1	B	124	ARG	NE-CZ-NH2	13.37	126.98	120.30
1	A	347	ASP	CB-CG-OD2	-12.22	107.30	118.30
1	B	82	LEU	CB-CG-CD1	11.60	130.72	111.00
1	B	328	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	B	382	ARG	CB-CG-CD	11.16	140.63	111.60
1	B	19	ARG	NE-CZ-NH2	11.01	125.80	120.30
1	A	192	ARG	NE-CZ-NH2	-10.87	114.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	A	122	LEU	CB-CG-CD2	10.24	128.41	111.00
1	B	122	LEU	CB-CG-CD2	9.73	127.53	111.00
1	B	346	LEU	CB-CG-CD1	9.49	127.13	111.00
1	A	233	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	A	175	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	A	240	GLU	OE1-CD-OE2	-9.27	112.18	123.30
1	B	143	LEU	CB-CG-CD2	8.96	126.23	111.00
1	A	124	ARG	NE-CZ-NH2	8.89	124.74	120.30
1	B	175	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	A	153	GLU	OE1-CD-OE2	-8.83	112.71	123.30
1	B	347	ASP	CB-CG-OD2	-8.80	110.38	118.30
1	B	52	PHE	CB-CG-CD1	8.77	126.94	120.80
1	A	279	ASP	CB-CG-OD2	8.74	126.17	118.30
1	A	311	ASP	CB-CG-OD2	-8.68	110.49	118.30
1	A	199	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	157	ARG	NE-CZ-NH1	-8.34	116.13	120.30
1	B	263	ARG	NE-CZ-NH1	-8.23	116.19	120.30
1	B	328	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	B	296	ASP	CB-CG-OD2	8.11	125.60	118.30
1	A	352	PHE	CB-CG-CD2	-8.05	115.16	120.80
1	B	199	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	51	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	A	335	ARG	CD-NE-CZ	7.77	134.48	123.60
1	A	48	ASP	CB-CG-OD1	7.64	125.18	118.30
1	A	59	ARG	NE-CZ-NH1	-7.43	116.59	120.30
1	B	279	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	335	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	B	263	ARG	NE-CZ-NH2	7.19	123.89	120.30
1	A	381	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	B	148	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	192	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	B	51	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	B	72	ASP	CB-CA-C	-7.01	96.37	110.40
1	A	4	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	A	240	GLU	CG-CD-OE1	6.91	132.11	118.30
1	B	391	VAL	CG1-CB-CG2	6.87	121.89	110.90
1	B	311	ASP	CB-CG-OD1	6.84	124.45	118.30
1	B	289	LEU	CB-CG-CD2	-6.78	99.47	111.00
1	B	153	GLU	OE1-CD-OE2	-6.75	115.20	123.30
1	A	82	LEU	CB-CG-CD2	6.73	122.44	111.00
1	B	1	ASP	CB-CG-OD2	-6.58	112.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	B	87	GLU	OE1-CD-OE2	-6.49	115.51	123.30
1	B	399	VAL	CG1-CB-CG2	-6.48	100.53	110.90
1	B	308	VAL	CG1-CB-CG2	-6.44	100.59	110.90
1	B	436	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	166	GLU	CB-CG-CD	-6.35	97.06	114.20
1	B	124	ARG	NH1-CZ-NH2	-6.34	112.42	119.40
1	A	167	THR	CB-CA-C	6.33	128.70	111.60
1	B	283	ARG	NE-CZ-NH2	6.31	123.46	120.30
1	A	339	GLU	OE1-CD-OE2	-6.30	115.74	123.30
1	A	263	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	A	4	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	B	240	GLU	OE1-CD-OE2	-6.20	115.86	123.30
1	A	284	GLU	CB-CG-CD	-6.06	97.85	114.20
1	B	367	TYR	CD1-CE1-CZ	-6.05	114.36	119.80
1	B	279	ASP	OD1-CG-OD2	-5.99	111.91	123.30
1	B	70	ARG	NE-CZ-NH2	5.99	123.29	120.30
1	B	200	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	163	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	192	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	48	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	B	341	THR	OG1-CB-CG2	5.91	123.60	110.00
1	B	200	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	B	266	LEU	CB-CG-CD1	5.86	120.97	111.00
1	B	1	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	367	TYR	CD1-CE1-CZ	-5.83	114.55	119.80
1	B	52	PHE	CB-CG-CD2	-5.81	116.73	120.80
1	A	373	TYR	CD1-CE1-CZ	-5.79	114.59	119.80
1	B	74	GLY	N-CA-C	-5.69	98.87	113.10
1	B	373	TYR	CD1-CE1-CZ	-5.63	114.73	119.80
1	B	282	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	B	295	GLU	CG-CD-OE1	-5.57	107.16	118.30
1	B	339	GLU	OE1-CD-OE2	-5.51	116.69	123.30
1	B	381	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	429	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	15	PRO	N-CD-CG	-5.43	95.05	103.20
1	A	52	PHE	CB-CG-CD2	5.43	124.60	120.80
1	B	246	LEU	CB-CG-CD2	5.42	120.21	111.00
1	B	283	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	A	19	ARG	NH1-CZ-NH2	-5.40	113.46	119.40
1	B	233	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	279	ASP	CB-CG-OD2	5.37	123.13	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	-2	SER	N-CA-CB	5.36	118.53	110.50
1	B	82	LEU	CB-CG-CD2	5.35	120.10	111.00
1	A	227	THR	O-C-N	-5.34	114.11	123.20
1	A	410	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	169	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	23	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	379	GLU	OE1-CD-OE2	-5.26	116.99	123.30
1	B	37	TRP	CD1-NE1-CE2	-5.24	104.28	109.00
1	B	335	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	B	343	ASP	CB-CG-OD1	5.23	123.00	118.30
1	B	4	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	457	ARG	N-CA-CB	5.13	119.84	110.60
1	B	352	PHE	CB-CG-CD2	-5.13	117.21	120.80
1	B	166	GLU	O-C-N	5.11	130.88	122.70
1	B	124	ARG	CD-NE-CZ	-5.08	116.49	123.60
1	B	175	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	447	GLU	OE1-CD-OE2	-5.08	117.21	123.30
1	B	236	ARG	CG-CD-NE	5.06	122.43	111.80
1	A	72	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	GLY	Mainchain,Peptide
1	A	280	ALA	Mainchain
1	B	72	ASP	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	3422	0	3387	51	0
1	B	3406	0	3375	60	0
2	A	48	0	26	6	0
2	B	48	0	26	8	0
3	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	227	0	0	5	0
4	B	247	0	0	12	0
All	All	7404	0	6822	114	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 8.

All (114) 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)
2:A:476:NDP:C5N	4:A:587:HOH:O	1.84	1.21
2:A:476:NDP:H5N	4:A:587:HOH:O	1.38	1.19
2:B:476:NDP:C5N	4:B:533:HOH:O	1.93	1.15
1:B:262:LEU:O	1:B:266:LEU:HD13	1.53	1.08
2:B:476:NDP:H5N	4:B:533:HOH:O	1.55	1.05
1:A:11:ARG:HG3	1:A:11:ARG:HH21	1.18	1.03
1:A:70:ARG:HH21	1:A:70:ARG:HG3	1.27	0.99
1:B:262:LEU:HD23	1:B:266:LEU:CD1	1.96	0.95
1:B:72:ASP:O	1:B:73:GLU:HG2	1.67	0.95
1:A:90:HIS:HD2	1:A:92:ASP:H	1.14	0.90
1:A:131:ARG:HH21	1:B:131:ARG:HH12	1.22	0.88
1:B:391:VAL:HG21	1:B:428:LEU:HD13	1.57	0.86
2:B:476:NDP:O7N	4:B:594:HOH:O	1.95	0.84
1:A:341:THR:HA	1:A:344:LEU:HD13	1.59	0.83
1:B:262:LEU:HD23	1:B:266:LEU:HD13	1.59	0.82
1:B:262:LEU:HD23	1:B:266:LEU:HD11	1.63	0.81
1:A:11:ARG:NH2	1:A:11:ARG:HG3	1.90	0.77
1:A:335:ARG:CB	1:A:335:ARG:HH21	1.97	0.77
1:A:166:GLU:N	1:A:166:GLU:OE2	2.18	0.76
1:B:344:LEU:HB2	1:B:346:LEU:CD1	2.17	0.75
1:A:245:HIS:HE1	1:A:274:THR:OG1	1.70	0.74
1:A:335:ARG:HB3	1:A:335:ARG:HH21	1.51	0.74
1:B:393:TRP:HB2	2:B:476:NDP:C5N	2.17	0.73
1:A:203:HIS:HD2	4:A:553:HOH:O	1.72	0.73
1:B:208:VAL:HG23	1:B:211:SER:OG	1.91	0.71
1:B:41:VAL:CG2	1:B:164:LEU:HD11	2.21	0.71
1:B:299:LEU:HD23	1:B:300:THR:N	2.06	0.71
1:A:131:ARG:NH2	1:B:131:ARG:HH12	1.88	0.71
2:B:476:NDP:H41N	4:B:533:HOH:O	1.92	0.70
1:A:90:HIS:CD2	1:A:92:ASP:H	2.04	0.69
1:B:469:VAL:HG21	4:B:535:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:CG	1:A:11:ARG:HH21	1.98	0.68
1:B:410:ARG:NH1	4:B:565:HOH:O	2.25	0.68
1:B:32:HIS:HE1	4:B:561:HOH:O	1.76	0.68
1:A:70:ARG:HH21	1:A:70:ARG:CG	2.03	0.67
1:A:393:TRP:HB2	2:A:476:NDP:C5N	2.24	0.67
1:A:203:HIS:HE1	1:A:467:GLU:OE2	1.76	0.67
1:B:245:HIS:HE1	1:B:274:THR:OG1	1.79	0.66
1:B:391:VAL:HG21	1:B:428:LEU:CD1	2.25	0.65
1:B:344:LEU:HB2	1:B:346:LEU:HD12	1.77	0.65
1:B:262:LEU:CD2	1:B:266:LEU:HD11	2.27	0.64
1:B:466:PRO:O	1:B:469:VAL:HG22	1.98	0.64
1:A:391:VAL:HG22	1:A:431:MET:SD	2.40	0.62
2:A:476:NDP:H41N	4:A:587:HOH:O	1.92	0.60
1:A:70:ARG:NH2	1:A:70:ARG:HG3	2.07	0.59
1:A:77:HIS:HE1	1:A:180:LEU:O	1.86	0.58
1:A:220:SER:OG	1:A:245:HIS:HD2	1.85	0.58
1:A:233:ARG:NE	1:A:236:ARG:HH21	2.01	0.58
2:A:476:NDP:C4N	4:A:587:HOH:O	2.26	0.58
1:A:11:ARG:NH1	1:A:194:SER:O	2.38	0.57
1:A:135:LEU:O	1:A:380:HIS:HD2	1.88	0.56
2:B:476:NDP:C4N	4:B:533:HOH:O	2.31	0.56
1:B:135:LEU:O	1:B:380:HIS:HD2	1.90	0.55
1:A:335:ARG:HB2	1:A:335:ARG:HH21	1.71	0.54
1:A:131:ARG:HH21	1:B:131:ARG:NH1	2.00	0.54
1:B:299:LEU:C	1:B:299:LEU:HD23	2.27	0.53
1:A:131:ARG:NH2	1:B:131:ARG:NH1	2.56	0.53
1:B:19:ARG:NH1	4:B:539:HOH:O	2.36	0.53
1:B:77:HIS:HE1	1:B:180:LEU:O	1.91	0.53
1:B:413:ARG:HG3	1:B:413:ARG:NH1	2.22	0.53
1:A:124:ARG:H	1:A:140:GLN:NE2	2.07	0.52
1:B:72:ASP:O	1:B:73:GLU:CG	2.48	0.52
1:A:11:ARG:HH22	1:A:195:GLY:HA3	1.75	0.52
1:B:41:VAL:CG2	1:B:164:LEU:CD1	2.88	0.51
1:B:382:ARG:HD3	1:B:388:ALA:O	2.11	0.51
1:B:466:PRO:O	1:B:469:VAL:CG2	2.59	0.51
1:B:41:VAL:HG21	1:B:164:LEU:HD11	1.91	0.50
1:A:224:THR:OG1	1:A:304:HIS:HD2	1.94	0.50
1:B:394:GLY:O	2:B:476:NDP:H42N	2.12	0.49
1:B:236:ARG:HD3	1:B:265:GLU:OE2	2.13	0.49
1:B:262:LEU:CD2	1:B:266:LEU:CD1	2.79	0.49
1:A:57:THR:OG1	1:A:90:HIS:HE1	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLU:N	1:A:166:GLU:CD	2.66	0.48
1:B:310:HIS:HD2	1:B:311:ASP:OD2	1.96	0.48
1:B:59:ARG:HB2	1:B:105:LEU:HD12	1.95	0.47
1:B:6:HIS:CE1	1:B:8:GLU:OE1	2.68	0.47
1:B:37:TRP:CE3	1:B:164:LEU:HD12	2.50	0.47
1:B:413:ARG:HG3	1:B:413:ARG:HH11	1.79	0.47
1:B:391:VAL:HG22	1:B:431:MET:SD	2.54	0.47
1:B:353:SER:O	2:B:476:NDP:H6N	2.15	0.47
1:A:70:ARG:CG	1:A:70:ARG:NH2	2.72	0.47
1:B:220:SER:OG	1:B:245:HIS:HD2	1.98	0.46
1:A:171:ARG:HE	1:A:171:ARG:HB2	1.65	0.46
1:B:125:GLY:HA2	4:B:629:HOH:O	2.16	0.46
1:A:224:THR:OG1	1:A:304:HIS:CD2	2.69	0.46
1:B:387:THR:HG22	4:B:677:HOH:O	2.16	0.45
1:A:236:ARG:HD3	1:A:265:GLU:CD	2.36	0.45
1:A:138:PRO:HB2	1:A:373:TYR:CE1	2.52	0.45
1:A:394:GLY:O	2:A:476:NDP:H42N	2.16	0.45
1:A:304:HIS:HE1	1:A:329:ALA:O	2.00	0.44
1:A:236:ARG:HD3	1:A:265:GLU:OE2	2.18	0.44
1:A:-2:SER:H2	1:A:1:ASP:HB2	1.82	0.44
1:B:118:PRO:HG3	4:B:580:HOH:O	2.18	0.44
1:B:466:PRO:HA	1:B:469:VAL:HG22	1.97	0.44
1:B:299:LEU:C	1:B:299:LEU:CD2	2.86	0.44
1:B:469:VAL:HG23	1:B:470:SER:N	2.31	0.44
1:B:391:VAL:CG2	1:B:428:LEU:HD13	2.40	0.44
1:A:6:HIS:NE2	1:A:8:GLU:OE1	2.51	0.43
1:A:0:MET:SD	1:A:426:GLY:HA3	2.58	0.43
1:B:299:LEU:HD23	1:B:301:ALA:N	2.33	0.43
1:A:304:HIS:CE1	1:A:329:ALA:O	2.72	0.43
1:B:221:VAL:HG11	1:B:238:LEU:HD13	1.99	0.43
1:A:11:ARG:NH2	1:A:195:GLY:HA3	2.33	0.43
1:B:68:GLN:O	1:B:71:GLU:HB3	2.18	0.43
1:A:11:ARG:NH2	1:A:11:ARG:CG	2.62	0.42
1:A:341:THR:HB	1:A:346:LEU:HD11	2.01	0.42
1:B:59:ARG:HB2	1:B:105:LEU:CD1	2.49	0.42
1:A:208:VAL:HG11	1:B:11:ARG:NE	2.35	0.41
1:B:299:LEU:HD23	1:B:301:ALA:H	1.85	0.41
1:A:41:VAL:CG2	1:A:164:LEU:HD11	2.50	0.41
1:B:417:LEU:HD11	1:B:445:ASP:HB2	2.03	0.41
1:A:19:ARG:HB2	1:A:20:PRO:HD2	2.02	0.41
1:A:209:PRO:HD2	1:B:13:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ARG:CG	1:B:413:ARG:HH11	2.34	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	466/496 (94%)	454 (97%)	11 (2%)	1 (0%)	47 21
1	B	464/496 (94%)	452 (97%)	12 (3%)	0	100 100
All	All	930/992 (94%)	906 (97%)	23 (2%)	1 (0%)	51 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	GLY

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	329/351 (94%)	314 (95%)	15 (5%)	27 2
1	B	327/351 (93%)	311 (95%)	16 (5%)	25 2
All	All	656/702 (93%)	625 (95%)	31 (5%)	26 2

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	19	ARG
1	A	23	ARG
1	A	75	GLU
1	A	124	ARG
1	A	131	ARG
1	A	143	LEU
1	A	171	ARG
1	A	213	LYS
1	A	233	ARG
1	A	262	LEU
1	A	311	ASP
1	A	335	ARG
1	A	401	MET
1	A	410	ARG
1	B	-2	SER
1	B	6	HIS
1	B	23	ARG
1	B	48	ASP
1	B	82	LEU
1	B	124	ARG
1	B	131	ARG
1	B	208	VAL
1	B	213	LYS
1	B	262	LEU
1	B	266	LEU
1	B	295	GLU
1	B	299	LEU
1	B	401	MET
1	B	409	ASP
1	B	410	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) 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

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Mol	Chain	Res	Type
1	A	245	HIS
1	A	304	HIS
1	A	310	HIS
1	A	336	HIS
1	A	380	HIS
1	A	414	GLN
1	B	6	HIS
1	B	32	HIS
1	B	77	HIS
1	B	102	GLN
1	B	241	GLN
1	B	245	HIS
1	B	310	HIS
1	B	336	HIS
1	B	380	HIS

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	NDP	A	476	-	45,52,52	1.84	13 (28%)	53,80,80	1.86	12 (22%)
2	NDP	B	476	-	45,52,52	1.57	9 (20%)	53,80,80	1.84	13 (24%)
3	GOL	B	477	-	5,5,5	0.95	0	5,5,5	0.52	0

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	476	-	-	7/30/77/77	0/5/5/5
2	NDP	B	476	-	-	7/30/77/77	0/5/5/5
3	GOL	B	477	-	-	0/4/4/4	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	476	NDP	C4N-C3N	-4.80	1.40	1.49
2	B	476	NDP	O4B-C1B	4.67	1.47	1.41
2	A	476	NDP	P2B-O2B	3.72	1.66	1.59
2	A	476	NDP	C4A-N3A	3.46	1.40	1.35
2	A	476	NDP	C2A-N1A	3.33	1.40	1.33
2	B	476	NDP	C6N-C5N	3.29	1.39	1.33
2	A	476	NDP	C6N-C5N	3.08	1.38	1.33
2	B	476	NDP	C2A-N3A	3.07	1.37	1.32
2	A	476	NDP	C4N-C5N	-3.03	1.41	1.48
2	B	476	NDP	C4N-C3N	-3.02	1.44	1.49
2	B	476	NDP	C4A-N3A	2.83	1.39	1.35
2	B	476	NDP	P2B-O2B	2.78	1.64	1.59
2	A	476	NDP	C2N-C3N	2.75	1.42	1.34
2	A	476	NDP	C2A-N3A	2.68	1.36	1.32
2	A	476	NDP	O4B-C1B	2.62	1.44	1.41
2	B	476	NDP	C4N-C5N	-2.53	1.42	1.48
2	B	476	NDP	C3B-C4B	-2.37	1.46	1.53
2	B	476	NDP	C2A-N1A	2.21	1.38	1.33
2	A	476	NDP	PN-O2N	-2.18	1.45	1.55
2	A	476	NDP	C7N-C3N	2.16	1.53	1.48
2	A	476	NDP	C3B-C4B	-2.12	1.47	1.53
2	A	476	NDP	C1D-N1N	2.09	1.52	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	476	NDP	N3A-C2A-N1A	-5.48	120.12	128.68
2	B	476	NDP	O4B-C4B-C3B	5.06	115.12	105.11
2	A	476	NDP	O4B-C1B-C2B	-4.73	98.38	106.59
2	B	476	NDP	N3A-C2A-N1A	-4.58	121.52	128.68
2	B	476	NDP	C2A-N1A-C6A	3.96	125.52	118.75
2	A	476	NDP	C1B-N9A-C4A	-3.83	119.91	126.64
2	B	476	NDP	C4A-C5A-N7A	-3.79	105.45	109.40
2	A	476	NDP	O4B-C4B-C3B	3.60	112.23	105.11
2	B	476	NDP	O7N-C7N-C3N	-3.52	114.27	120.90
2	B	476	NDP	O4D-C4D-C3D	3.48	112.00	105.11
2	A	476	NDP	C1D-N1N-C6N	-3.26	113.81	120.83
2	A	476	NDP	C2D-C3D-C4D	3.08	108.63	102.64
2	A	476	NDP	C2A-N1A-C6A	3.07	124.01	118.75
2	B	476	NDP	C1D-N1N-C6N	-2.94	114.51	120.83
2	A	476	NDP	C4A-C5A-N7A	-2.83	106.45	109.40
2	A	476	NDP	C2B-C3B-C4B	-2.63	96.28	101.99
2	B	476	NDP	N6A-C6A-N1A	2.50	123.77	118.57
2	A	476	NDP	O2X-P2B-O1X	2.45	120.28	110.68
2	B	476	NDP	C3N-C2N-N1N	-2.34	119.75	123.10
2	B	476	NDP	C5A-C6A-N1A	-2.28	115.17	120.35
2	B	476	NDP	O2B-P2B-O1X	-2.25	100.70	109.39
2	B	476	NDP	C3N-C7N-N7N	2.23	121.62	117.67
2	A	476	NDP	C5B-C4B-C3B	2.17	123.31	115.18
2	B	476	NDP	O3B-C3B-C4B	-2.17	104.79	111.05
2	A	476	NDP	O2B-P2B-O1X	-2.08	101.35	109.39

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	476	NDP	C5D-O5D-PN-O1N
2	A	476	NDP	C5D-O5D-PN-O2N
2	B	476	NDP	C5D-O5D-PN-O2N
2	A	476	NDP	O4D-C1D-N1N-C6N
2	B	476	NDP	C5D-O5D-PN-O3
2	B	476	NDP	O4D-C1D-N1N-C6N
2	B	476	NDP	C5D-O5D-PN-O1N
2	B	476	NDP	O4B-C4B-C5B-O5B
2	A	476	NDP	PA-O3-PN-O2N
2	A	476	NDP	C5D-O5D-PN-O3
2	A	476	NDP	O4B-C4B-C5B-O5B
2	B	476	NDP	PA-O3-PN-O2N
2	A	476	NDP	C2N-C3N-C7N-N7N

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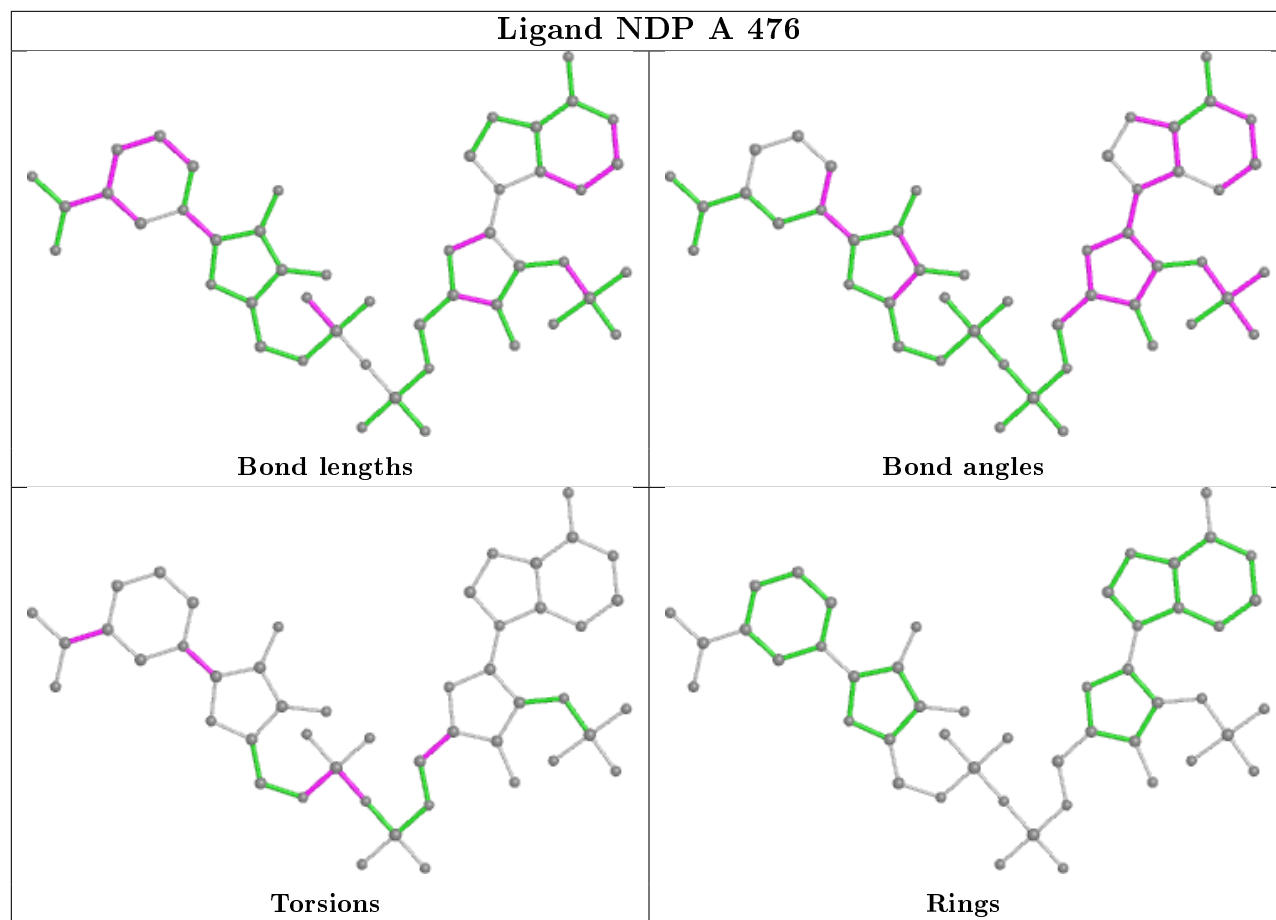
Mol	Chain	Res	Type	Atoms
2	B	476	NDP	C2N-C3N-C7N-N7N

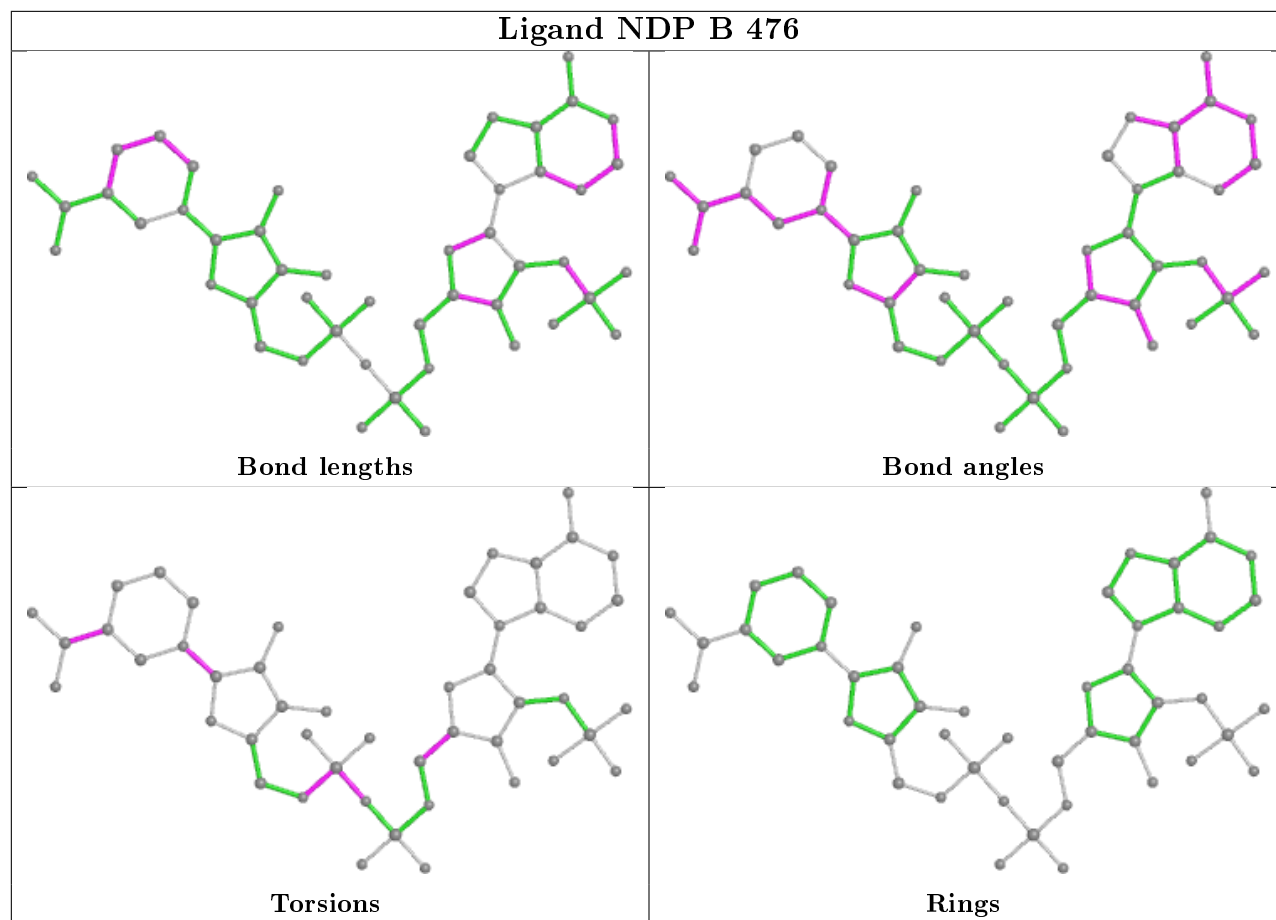
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	476	NDP	6	0
2	B	476	NDP	8	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	470/496 (94%)	0.81	50 (10%) 6 7	7, 14, 28, 42	0
1	B	468/496 (94%)	0.77	44 (9%) 8 10	6, 13, 28, 42	0
All	All	938/992 (94%)	0.79	94 (10%) 7 9	6, 14, 28, 42	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	399	VAL	8.5
1	A	413	ARG	7.6
1	B	410	ARG	7.5
1	A	410	ARG	6.9
1	B	401	MET	6.0
1	A	208	VAL	5.9
1	B	413	ARG	5.8
1	A	131	ARG	5.6
1	A	401	MET	5.5
1	B	131	ARG	5.4
1	B	399	VAL	5.2
1	A	-1	HIS	5.1
1	B	411	LEU	5.1
1	A	213	LYS	4.8
1	A	408	HIS	4.3
1	A	400	GLY	4.3
1	A	398	GLU	4.2
1	A	295	GLU	4.2
1	A	211	SER	4.0
1	A	11	ARG	3.9
1	B	213	LYS	3.9
1	B	21	ALA	3.9
1	A	209	PRO	3.9
1	B	72	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	411	LEU	3.8
1	B	412	VAL	3.8
1	B	91	THR	3.8
1	A	210	GLY	3.8
1	B	261	GLU	3.6
1	A	71	GLU	3.6
1	B	74	GLY	3.5
1	A	409	ASP	3.5
1	B	409	ASP	3.5
1	B	400	GLY	3.5
1	A	75	GLU	3.4
1	A	132	GLY	3.3
1	A	72	ASP	3.3
1	A	212	GLY	3.3
1	A	261	GLU	3.2
1	A	166	GLU	3.1
1	A	217	VAL	3.1
1	B	342	ALA	3.0
1	B	278	CYS	2.9
1	B	295	GLU	2.9
1	A	342	ALA	2.9
1	B	398	GLU	2.9
1	A	308	VAL	2.9
1	B	71	GLU	2.8
1	A	21	ALA	2.8
1	A	194	SER	2.7
1	B	264	ALA	2.6
1	A	412	VAL	2.6
1	B	69	LEU	2.6
1	B	440	ALA	2.5
1	A	122	LEU	2.5
1	B	268	GLN	2.5
1	B	343	ASP	2.5
1	A	268	GLN	2.4
1	A	161	LEU	2.4
1	B	-1	HIS	2.4
1	B	255	ASP	2.4
1	B	70	ARG	2.4
1	A	150	ILE	2.4
1	A	343	ASP	2.4
1	B	391	VAL	2.3
1	A	294	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	-2	SER	2.3
1	A	143	LEU	2.3
1	B	208	VAL	2.3
1	B	211	SER	2.3
1	A	216	PRO	2.2
1	A	352	PHE	2.2
1	B	62	TRP	2.2
1	A	73	GLU	2.2
1	B	75	GLU	2.2
1	B	369	ALA	2.2
1	B	280	ALA	2.2
1	B	150	ILE	2.2
1	B	166	GLU	2.2
1	B	352	PHE	2.1
1	A	414	GLN	2.1
1	A	257	PRO	2.1
1	B	267	GLU	2.1
1	A	228	GLY	2.1
1	A	391	VAL	2.1
1	A	130	GLY	2.1
1	B	45	LEU	2.1
1	B	122	LEU	2.1
1	A	74	GLY	2.0
1	B	68	GLN	2.0
1	A	311	ASP	2.0
1	B	23	ARG	2.0
1	A	296	ASP	2.0
1	B	143	LEU	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 carbohydrates in this entry.

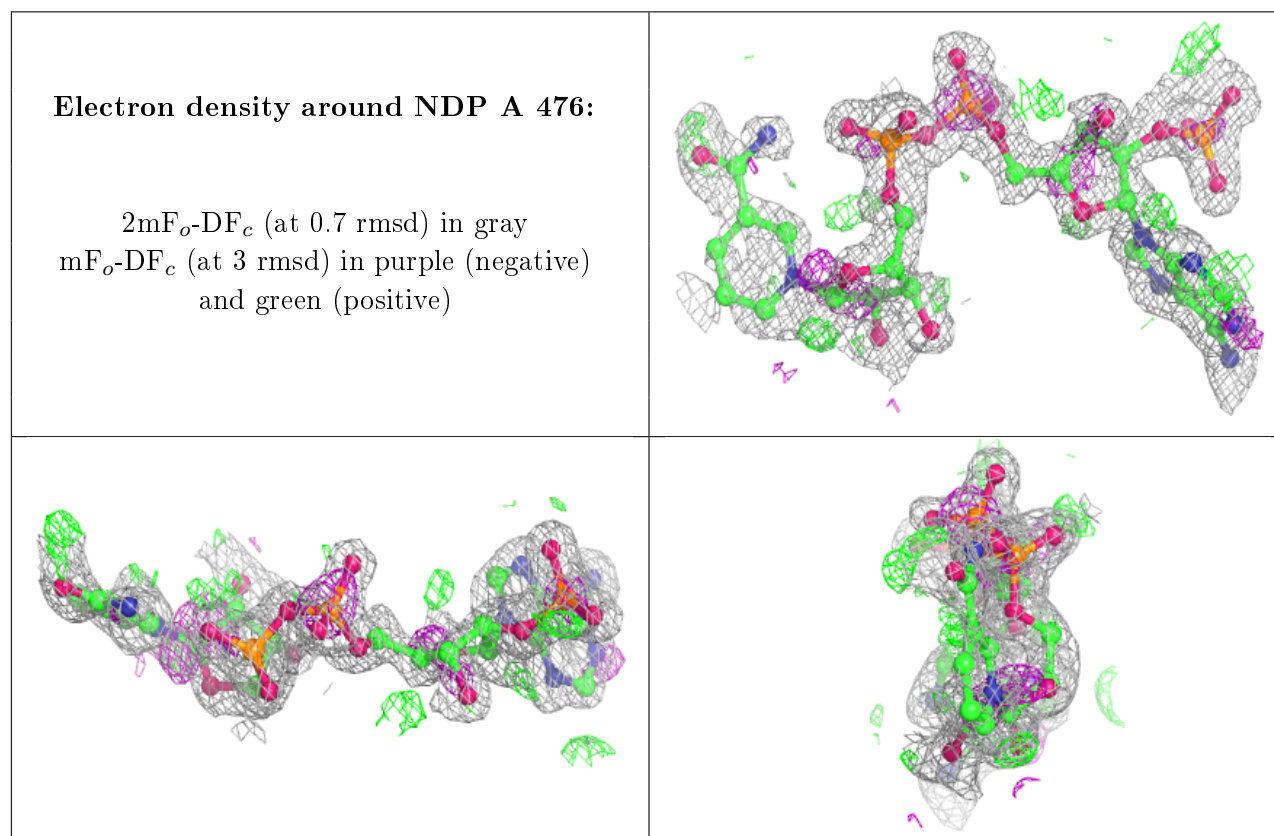
6.4 Ligands [i](#)

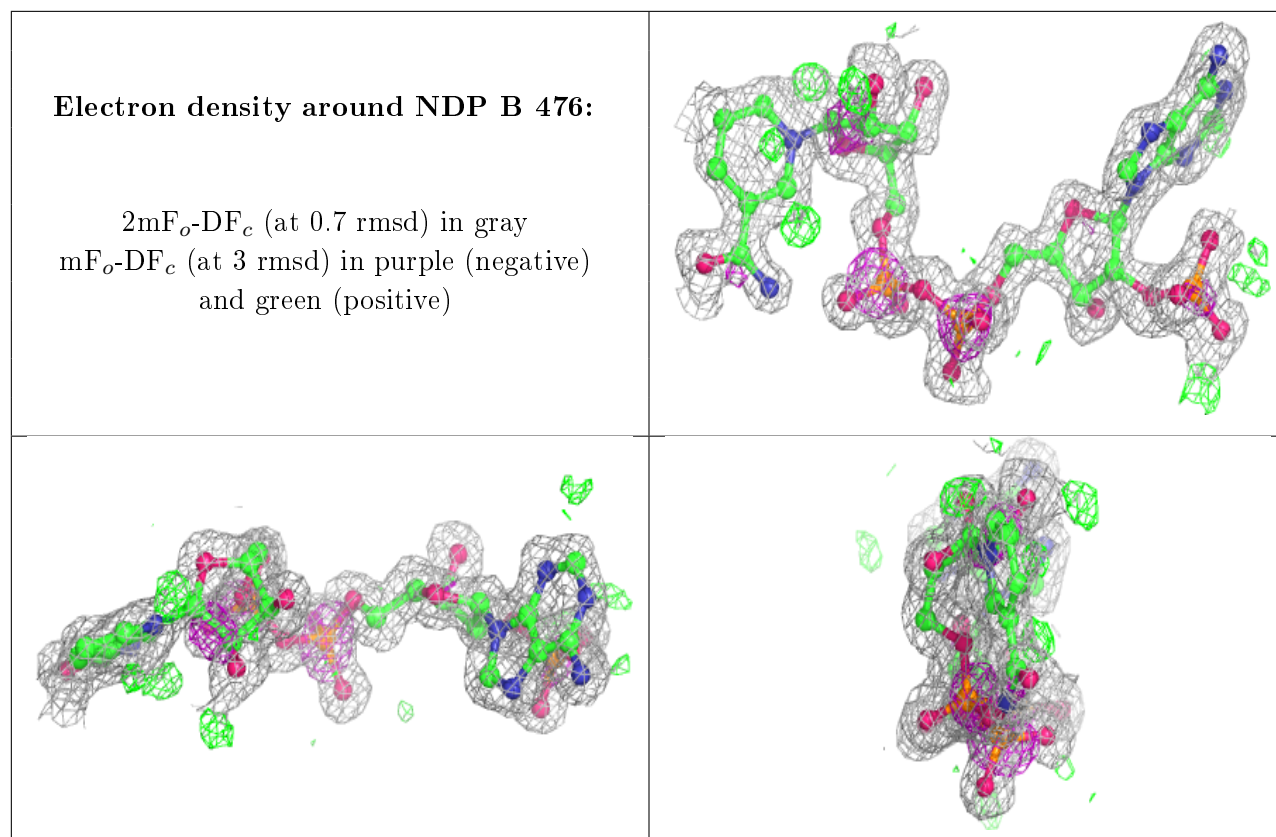
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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(\AA^2)	Q<0.9
2	NDP	A	476	48/48	0.91	0.22	18,23,36,38	0
2	NDP	B	476	48/48	0.93	0.17	14,19,23,27	0
3	GOL	B	477	6/6	0.93	0.10	15,17,18,18	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.