



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:50 PM UTC

PDB ID : 3MJV / pdb_00003mjv
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

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

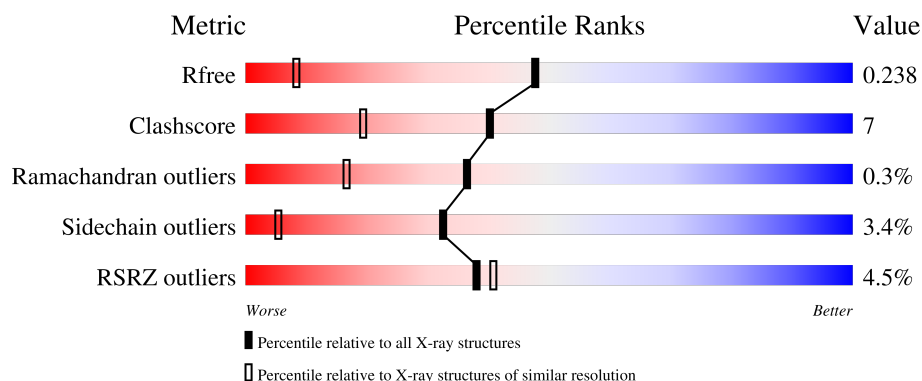
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.46 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}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (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 ≥ 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	5% 75% 18% • •
1	B	496	3% 78% 16% • •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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:

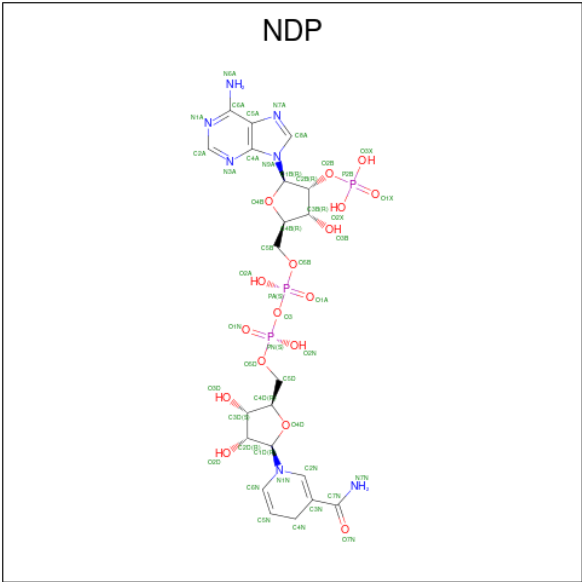
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q93NW7
A	-19	GLY	-	expression tag	UNP Q93NW7
A	-18	SER	-	expression tag	UNP Q93NW7
A	-17	SER	-	expression tag	UNP Q93NW7
A	-16	HIS	-	expression tag	UNP Q93NW7
A	-15	HIS	-	expression tag	UNP Q93NW7
A	-14	HIS	-	expression tag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

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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

- 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	0	0
			48	21	7	17		

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

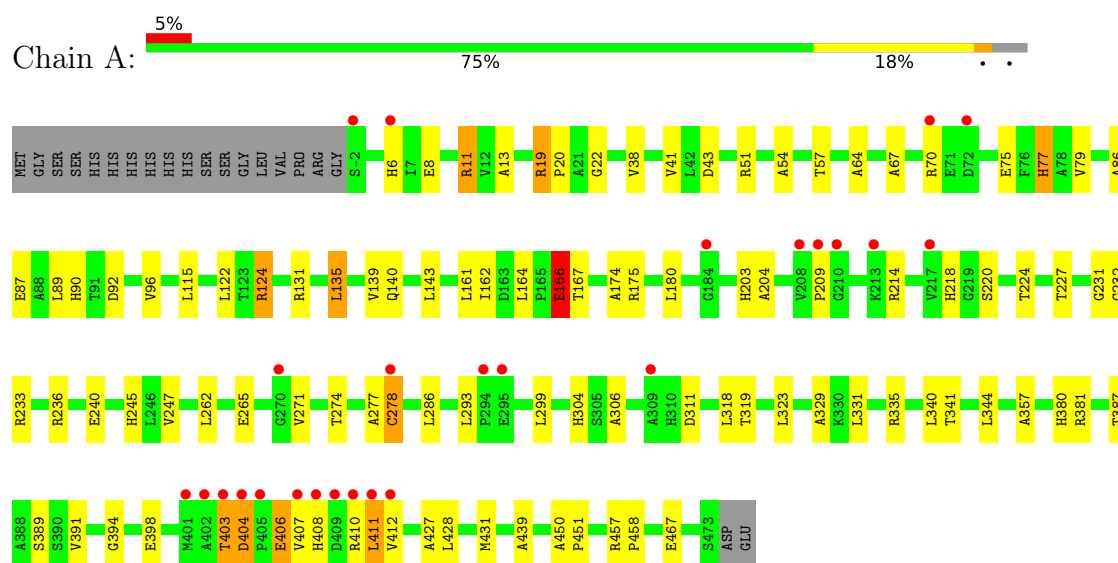
- Molecule 3 is water.

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

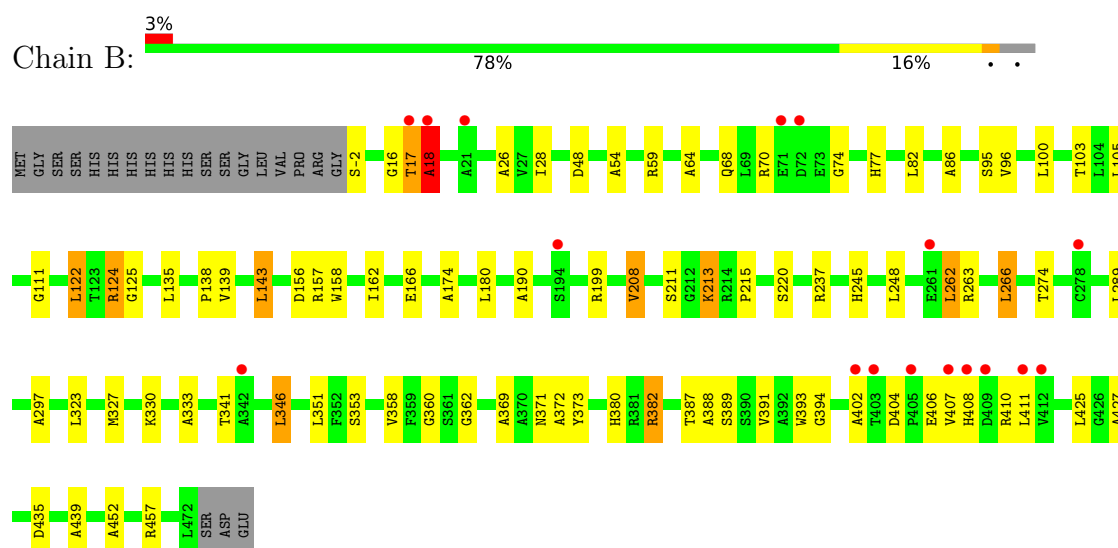
3 Residue-property plots [i](#)

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, α , β , γ	61.50Å 63.69Å 71.92Å 72.93° 67.21° 89.76°	Depositor
Resolution (Å)	50.00 – 1.46 50.00 – 1.46	Depositor EDS
% Data completeness (in resolution range)	82.9 (50.00-1.46) 82.9 (50.00-1.46)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.15%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	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 ²)	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.*

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	1.61	36/3531 (1.0%)	1.37	12/4822 (0.2%)
1	B	1.61	27/3525 (0.8%)	1.42	19/4814 (0.4%)
All	All	1.61	63/7056 (0.9%)	1.40	31/9636 (0.3%)

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	ARG	C-N	8.41	1.44	1.33
1	A	54	ALA	CA-CB	8.18	1.63	1.52
1	B	18	ALA	CA-CB	-7.84	1.40	1.53
1	A	96	VAL	CA-CB	-7.00	1.46	1.53
1	B	166	GLU	C-O	6.99	1.32	1.24
1	B	215	PRO	CA-C	6.77	1.55	1.51
1	A	13	ALA	N-CA	6.64	1.54	1.46
1	A	427	ALA	CA-CB	-6.40	1.43	1.53
1	B	95	SER	C-N	6.33	1.39	1.33
1	A	271	VAL	CA-CB	6.24	1.60	1.54
1	A	79	VAL	CA-CB	6.23	1.61	1.54
1	A	389	SER	N-CA	6.20	1.53	1.46
1	A	439	ALA	CA-C	-6.19	1.45	1.52
1	A	319	THR	CA-C	-6.12	1.44	1.53
1	B	86	ALA	CA-CB	6.09	1.61	1.52
1	B	26	ALA	CA-CB	-6.08	1.44	1.53
1	A	64	ALA	CA-CB	6.03	1.62	1.53
1	B	156	ASP	CA-C	-5.93	1.44	1.52
1	A	323	LEU	CA-C	5.76	1.60	1.52
1	B	54	ALA	CA-CB	5.74	1.60	1.52
1	B	199	ARG	C-O	5.72	1.30	1.23
1	A	387	THR	C-O	5.71	1.30	1.23
1	A	318	LEU	N-CA	5.70	1.53	1.46
1	B	330	LYS	C-O	5.69	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	LEU	N-CA	-5.65	1.39	1.46
1	B	28	ILE	C-O	5.65	1.29	1.24
1	B	333	ALA	CA-CB	-5.57	1.44	1.53
1	A	403	THR	CA-CB	5.50	1.59	1.52
1	A	96	VAL	N-CA	5.48	1.50	1.46
1	B	452	ALA	CA-CB	-5.48	1.44	1.53
1	A	175	ARG	N-CA	5.47	1.52	1.46
1	B	372	ALA	CA-CB	5.45	1.62	1.53
1	A	247	VAL	CA-CB	5.45	1.60	1.53
1	A	204	ALA	CA-CB	-5.43	1.44	1.53
1	A	457	ARG	CB-CG	-5.42	1.36	1.52
1	A	209	PRO	CA-C	5.39	1.59	1.52
1	B	208	VAL	CA-C	5.37	1.57	1.53
1	B	389	SER	N-CA	5.35	1.52	1.45
1	B	457	ARG	N-CA	-5.27	1.38	1.46
1	A	218	HIS	N-CA	5.26	1.52	1.46
1	A	227	THR	CA-C	5.26	1.59	1.52
1	A	231	GLY	N-CA	5.26	1.52	1.45
1	A	299	LEU	N-CA	5.25	1.52	1.46
1	B	158	TRP	CA-C	-5.25	1.46	1.52
1	A	38	VAL	C-O	5.25	1.29	1.24
1	B	362	GLY	N-CA	5.25	1.51	1.45
1	A	458	PRO	CA-CB	5.20	1.60	1.53
1	A	240	GLU	N-CA	5.20	1.52	1.46
1	A	357	ALA	CA-C	-5.19	1.45	1.52
1	A	135	LEU	CA-CB	5.17	1.59	1.52
1	B	111	GLY	N-CA	5.17	1.52	1.45
1	A	381	ARG	CB-CG	-5.17	1.36	1.52
1	A	43	ASP	N-CA	5.15	1.52	1.46
1	B	297	ALA	CA-CB	5.13	1.59	1.53
1	A	77	HIS	CA-CB	5.12	1.61	1.53
1	B	190	ALA	C-O	5.12	1.29	1.24
1	B	369	ALA	CA-CB	-5.10	1.45	1.53
1	A	278	CYS	N-CA	-5.10	1.39	1.46
1	B	124	ARG	NE-CZ	5.06	1.38	1.33
1	A	86	ALA	CA-CB	5.06	1.59	1.52
1	A	22	GLY	C-O	5.05	1.29	1.23
1	B	439	ALA	CA-C	-5.04	1.46	1.52
1	B	96	VAL	CA-CB	-5.01	1.48	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	ARG	NE-CZ-NH1	11.02	132.52	121.50
1	B	382	ARG	NE-CZ-NH2	-10.08	110.13	119.20
1	B	382	ARG	CB-CG-CD	9.84	133.94	111.30
1	B	391	VAL	CB-CA-C	-8.99	99.30	110.99
1	B	382	ARG	CD-NE-CZ	8.89	136.85	124.40
1	A	232	GLY	N-CA-C	7.83	122.38	112.83
1	A	174	ALA	N-CA-C	-7.30	102.71	111.69
1	A	214	ARG	CA-C-N	-7.11	113.06	120.38
1	A	214	ARG	C-N-CA	-7.11	113.06	120.38
1	A	167	THR	CB-CA-C	6.82	121.37	110.19
1	B	391	VAL	CA-CB-CG2	6.52	121.48	110.40
1	B	358	VAL	CB-CA-C	6.40	120.41	112.02
1	B	457	ARG	CA-C-N	-6.38	114.06	120.31
1	B	457	ARG	C-N-CA	-6.38	114.06	120.31
1	B	74	GLY	N-CA-C	-6.32	100.80	112.62
1	B	360	GLY	N-CA-C	-6.30	104.86	112.48
1	A	293	LEU	N-CA-C	6.18	117.49	109.64
1	B	70	ARG	O-C-N	5.98	128.97	122.15
1	A	19	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	A	51	ARG	NE-CZ-NH1	-5.56	115.94	121.50
1	A	166	GLU	CA-C-N	-5.52	115.32	123.05
1	A	166	GLU	C-N-CA	-5.52	115.32	123.05
1	B	68	GLN	N-CA-C	5.35	116.79	111.07
1	B	64	ALA	N-CA-C	5.32	117.07	111.28
1	B	157	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	A	412	VAL	N-CA-C	5.22	115.43	110.42
1	A	19	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	B	427	ALA	N-CA-C	-5.16	105.73	111.36
1	B	122	LEU	CB-CG-CD2	5.16	126.17	110.70
1	B	263	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	B	263	ARG	NE-CZ-NH1	-5.01	116.49	121.50

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	49	0
1	B	3456	0	3420	43	0
2	A	48	0	25	1	0
2	B	48	0	25	2	0
3	A	254	0	0	5	0
3	B	279	0	0	6	0
All	All	7547	0	6895	92	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 7.

All (92) 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:16:GLY:O	1:B:17:THR:C	2.25	0.80
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: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:B:262:LEU:C	1:B:262:LEU:HD23	2.20	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:A:166:GLU:H	1:A:166:GLU:CD	2.06	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:398:GLU:C	1:A:403:THR:HG21	2.37	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:262:LEU:C	1:B:262:LEU:CD2	2.90	0.43
1:A:331:LEU:C	1:A:331:LEU:HD23	2.44	0.42
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 [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	474/496 (96%)	458 (97%)	15 (3%)	1 (0%)	43	21
1	B	473/496 (95%)	462 (98%)	9 (2%)	2 (0%)	30	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	947/992 (96%)	920 (97%)	24 (2%)	3 (0%)	36	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLU
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%)	323 (97%)	11 (3%)	33	6
1	B	333/351 (95%)	321 (96%)	12 (4%)	31	5
All	All	667/702 (95%)	644 (97%)	23 (3%)	32	5

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	75	GLU
1	A	124	ARG
1	A	131	ARG
1	A	143	LEU
1	A	166	GLU
1	A	262	LEU
1	A	265	GLU
1	A	311	ASP
1	A	404	ASP
1	A	411	LEU
1	B	-2	SER
1	B	48	ASP
1	B	82	LEU
1	B	124	ARG

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Mol	Chain	Res	Type
1	B	143	LEU
1	B	213	LYS
1	B	262	LEU
1	B	266	LEU
1	B	289	LEU
1	B	346	LEU
1	B	406	GLU
1	B	410	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	10	ASN
1	A	65	GLN
1	A	68	GLN
1	A	77	HIS
1	A	90	HIS
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	A	423	HIS
1	B	32	HIS
1	B	65	GLN
1	B	68	GLN
1	B	77	HIS
1	B	245	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 [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	B	476	-	51,52,52	1.55	8 (15%)	71,80,80	2.22	21 (29%)
2	NDP	A	476	-	51,52,52	1.67	10 (19%)	71,80,80	1.97	18 (25%)

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	8/34/77/77	0/5/5/5
2	NDP	A	476	-	1/1/14/17	8/34/77/77	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	476	NDP	PA-O3	5.48	1.65	1.59
2	A	476	NDP	PA-O3	5.02	1.64	1.59
2	A	476	NDP	C4N-C3N	-4.64	1.41	1.50
2	A	476	NDP	P2B-O2B	3.92	1.66	1.59
2	B	476	NDP	C4A-N3A	3.73	1.41	1.34
2	B	476	NDP	C4N-C5N	-3.13	1.40	1.49
2	B	476	NDP	P2B-O2B	3.12	1.65	1.59
2	A	476	NDP	C4N-C5N	-3.09	1.41	1.49
2	B	476	NDP	C4N-C3N	-3.09	1.44	1.50
2	A	476	NDP	C8A-N7A	2.97	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	476	NDP	O7N-C7N	-2.85	1.17	1.24
2	A	476	NDP	C5A-N7A	-2.67	1.34	1.39
2	A	476	NDP	O4D-C1D	2.46	1.47	1.42
2	B	476	NDP	C8A-N7A	2.26	1.36	1.31
2	A	476	NDP	C6N-N1N	-2.22	1.31	1.37
2	A	476	NDP	C1D-N1N	2.12	1.52	1.46
2	A	476	NDP	C6N-C5N	2.11	1.39	1.33
2	B	476	NDP	O4D-C1D	2.04	1.46	1.42

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	476	NDP	C2B-C3B-C4B	-7.45	85.97	101.99
2	A	476	NDP	C2B-C3B-C4B	-7.01	86.93	101.99
2	B	476	NDP	N3A-C2A-N1A	-6.43	118.84	128.58
2	A	476	NDP	O4B-C4B-C3B	5.51	116.09	105.15
2	B	476	NDP	C2A-N1A-C6A	5.27	127.39	118.73
2	A	476	NDP	N3A-C2A-N1A	-4.89	121.18	128.58
2	B	476	NDP	O4B-C4B-C3B	4.46	114.01	105.15
2	B	476	NDP	C5B-C4B-C3B	3.75	128.71	115.21
2	B	476	NDP	O2B-P2B-O1X	-3.63	96.41	109.33
2	B	476	NDP	N9A-C8A-N7A	-3.49	108.98	113.94
2	B	476	NDP	O7N-C7N-C3N	-3.43	114.43	120.90
2	B	476	NDP	C6A-C5A-N7A	3.32	138.49	132.09
2	A	476	NDP	C5A-C4A-N9A	3.31	109.42	105.81
2	B	476	NDP	C4B-O4B-C1B	-3.28	102.22	109.47
2	A	476	NDP	C4B-O4B-C1B	-3.14	102.53	109.47
2	A	476	NDP	O3B-C3B-C4B	3.09	119.96	111.08
2	A	476	NDP	C5B-C4B-C3B	3.06	126.21	115.21
2	B	476	NDP	C5A-N7A-C8A	3.01	108.17	103.45
2	B	476	NDP	C6A-C5A-C4A	-2.97	113.13	117.18
2	B	476	NDP	O4B-C1B-C2B	-2.94	101.52	106.59
2	A	476	NDP	C2A-N1A-C6A	2.94	123.56	118.73
2	B	476	NDP	O3B-C3B-C4B	2.85	119.26	111.08
2	B	476	NDP	C3N-C7N-N7N	2.80	122.64	117.67
2	B	476	NDP	C4A-N9A-C1B	-2.69	120.34	126.63
2	A	476	NDP	O2B-P2B-O1X	-2.69	99.75	109.33
2	B	476	NDP	C1D-N1N-C6N	-2.67	115.12	120.77
2	A	476	NDP	N9A-C8A-N7A	-2.67	110.15	113.94
2	A	476	NDP	C4A-C5A-N7A	-2.66	107.54	110.58
2	A	476	NDP	O4B-C4B-C5B	2.61	117.69	109.33
2	A	476	NDP	C5A-C4A-N3A	-2.60	123.14	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	476	NDP	O2N-PN-O3	2.55	114.17	107.27
2	B	476	NDP	C1B-N9A-C8A	2.46	132.56	127.09
2	A	476	NDP	C2A-N3A-C4A	2.44	117.79	111.83
2	B	476	NDP	O3X-P2B-O2X	2.29	116.40	107.80
2	B	476	NDP	O2A-PA-O1A	2.27	122.99	112.44
2	A	476	NDP	C1B-N9A-C8A	2.17	131.90	127.09
2	A	476	NDP	C5A-N7A-C8A	2.09	106.74	103.45
2	A	476	NDP	O4B-C1B-C2B	-2.09	102.99	106.59
2	B	476	NDP	O4B-C4B-C5B	2.00	115.76	109.33

All (2) chirality outliers are listed below:

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

All (16) torsion outliers are listed below:

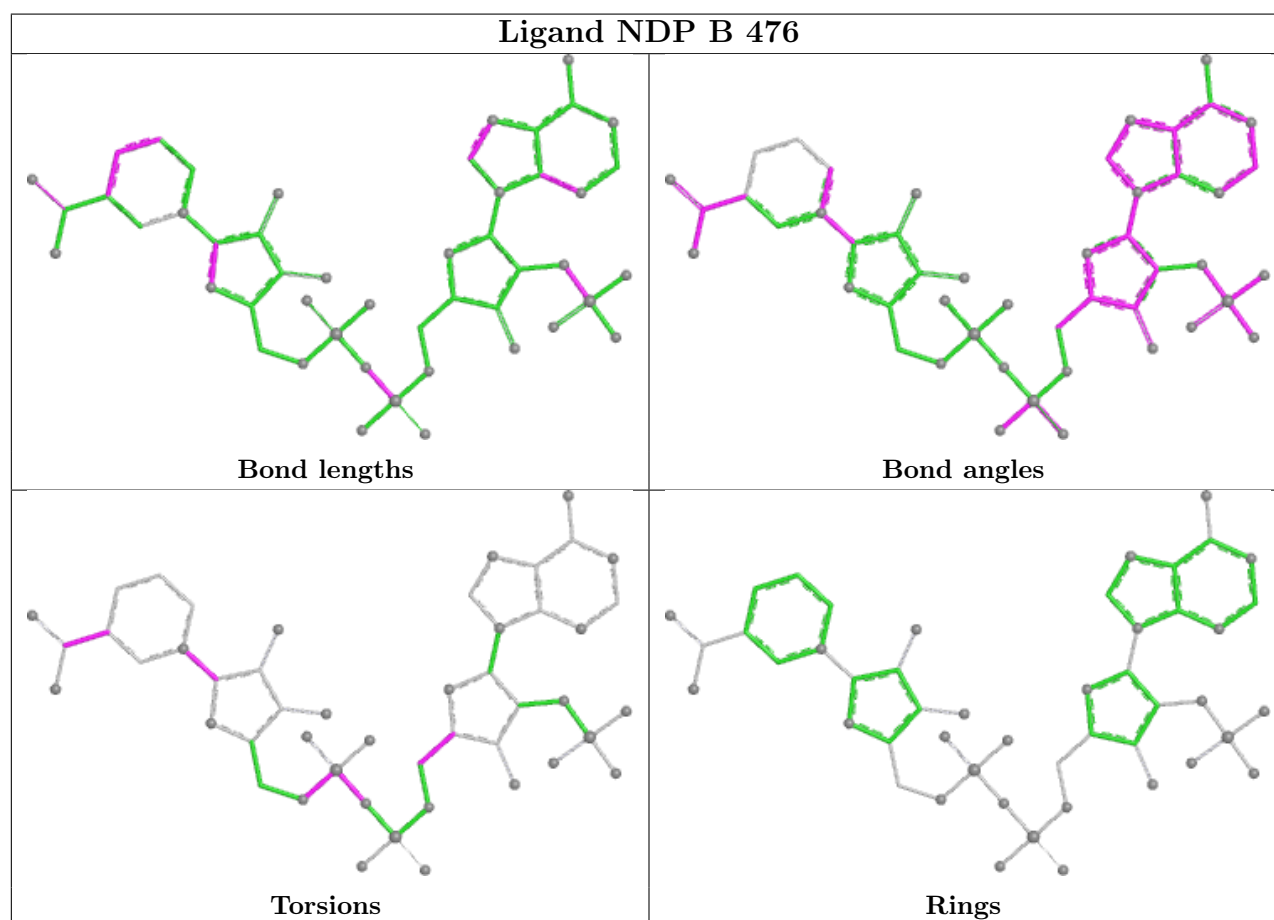
Mol	Chain	Res	Type	Atoms
2	A	476	NDP	C5D-O5D-PN-O3
2	A	476	NDP	C5D-O5D-PN-O2N
2	B	476	NDP	C5D-O5D-PN-O3
2	B	476	NDP	C5D-O5D-PN-O1N
2	B	476	NDP	C5D-O5D-PN-O2N
2	B	476	NDP	C3B-C4B-C5B-O5B
2	A	476	NDP	O4D-C1D-N1N-C6N
2	B	476	NDP	O4B-C4B-C5B-O5B
2	A	476	NDP	O4B-C4B-C5B-O5B
2	B	476	NDP	O4D-C1D-N1N-C6N
2	A	476	NDP	C3B-C4B-C5B-O5B
2	A	476	NDP	C5D-O5D-PN-O1N
2	B	476	NDP	PA-O3-PN-O2N
2	B	476	NDP	C2N-C3N-C7N-N7N
2	A	476	NDP	PA-O3-PN-O2N
2	A	476	NDP	PA-O3-PN-O1N

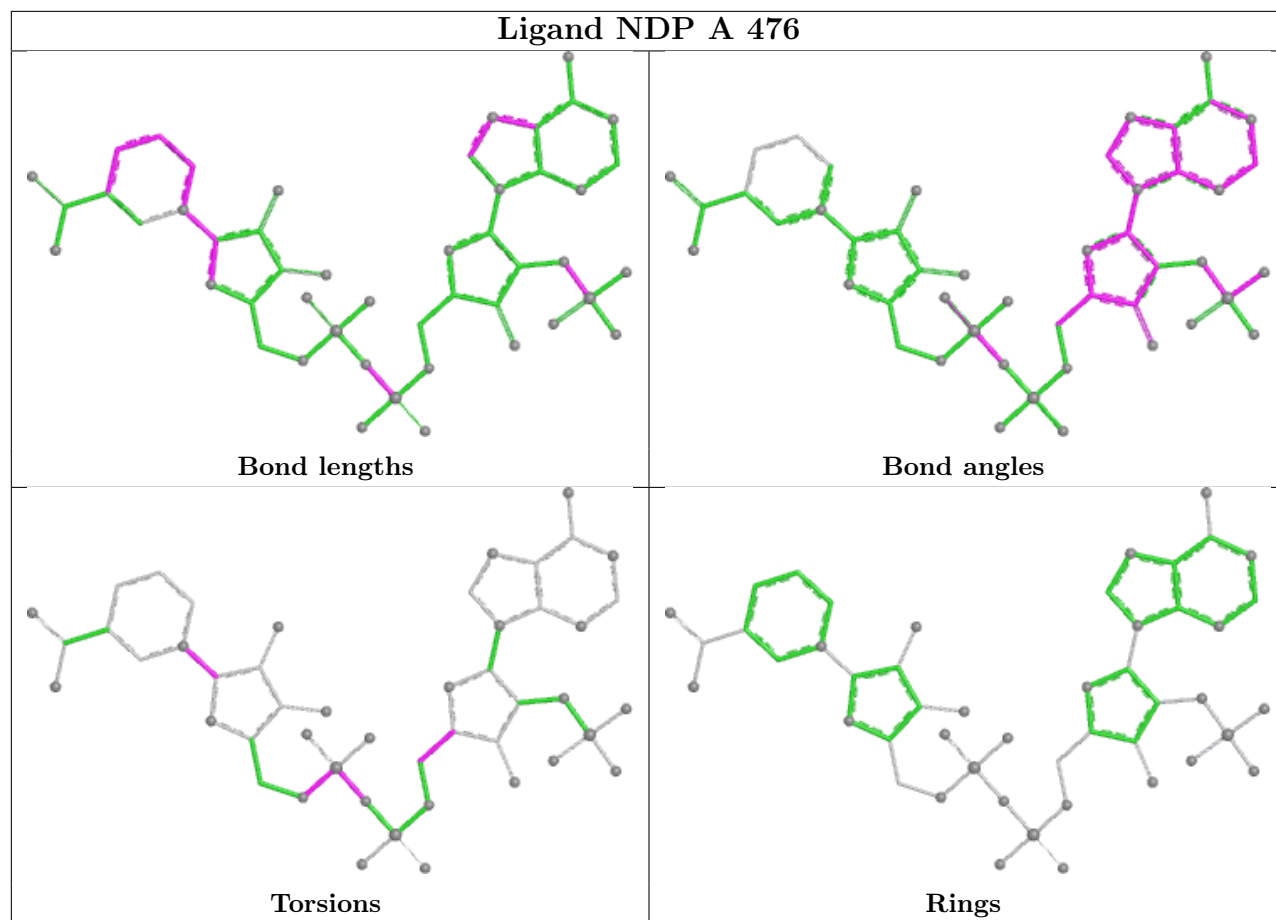
There are no ring outliers.

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, 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	476/496 (95%)	0.44	26 (5%) 30 30	9, 16, 32, 67	0
1	B	475/496 (95%)	0.36	17 (3%) 46 48	8, 15, 30, 64	0
All	All	951/992 (95%)	0.40	43 (4%) 38 41	8, 16, 32, 67	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	402	ALA	6.8
1	B	411	LEU	5.7
1	A	407	VAL	5.5
1	B	18	ALA	5.5
1	B	17	THR	4.9
1	A	411	LEU	4.1
1	A	209	PRO	4.1
1	B	405	PRO	4.1
1	A	404	ASP	4.0
1	A	405	PRO	3.8
1	A	403	THR	3.7
1	B	402	ALA	3.7
1	B	407	VAL	3.6
1	A	208	VAL	3.2
1	B	412	VAL	3.1
1	B	403	THR	3.1
1	A	412	VAL	3.0
1	A	-2	SER	2.9
1	A	184	GLY	2.9
1	A	401	MET	2.9
1	A	410	ARG	2.9
1	A	295	GLU	2.8
1	A	217	VAL	2.7
1	B	342	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	72	ASP	2.6
1	A	278	CYS	2.5
1	A	70	ARG	2.5
1	B	278	CYS	2.4
1	A	408	HIS	2.4
1	B	21	ALA	2.4
1	A	270	GLY	2.4
1	A	6	HIS	2.3
1	B	409	ASP	2.3
1	B	71	GLU	2.3
1	B	261	GLU	2.2
1	A	213	LYS	2.1
1	A	294	PRO	2.1
1	B	194	SER	2.1
1	A	72	ASP	2.1
1	A	409	ASP	2.1
1	B	408	HIS	2.1
1	A	210	GLY	2.1
1	A	309	ALA	2.1

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.

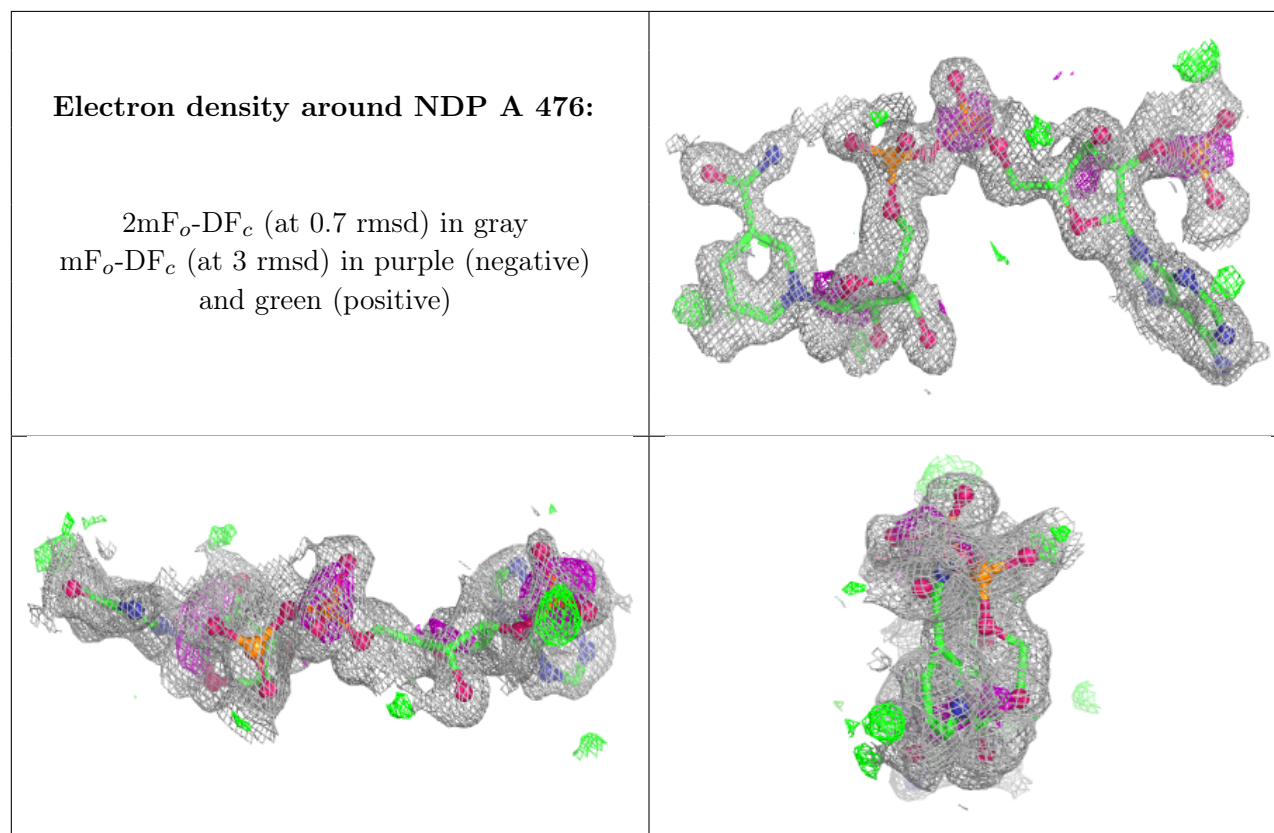
6.4 Ligands [i](#)

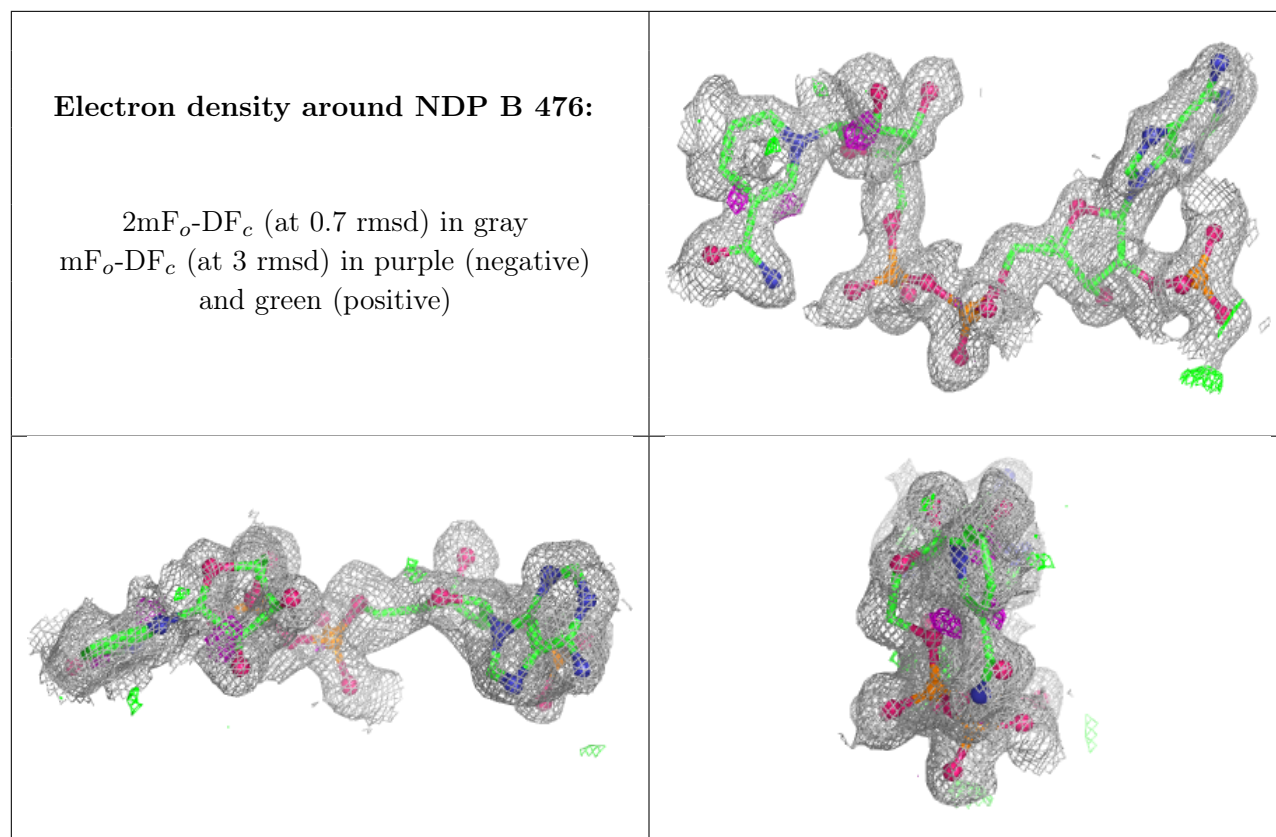
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NDP	A	476	48/48	0.94	0.08	16,21,25,25	0
2	NDP	B	476	48/48	0.97	0.06	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.