Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2025 – 05:50 AM EDT

PDB ID	:	3MJE / pdb_00003mje
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 (i) 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 (i)) were used in the production of this report:

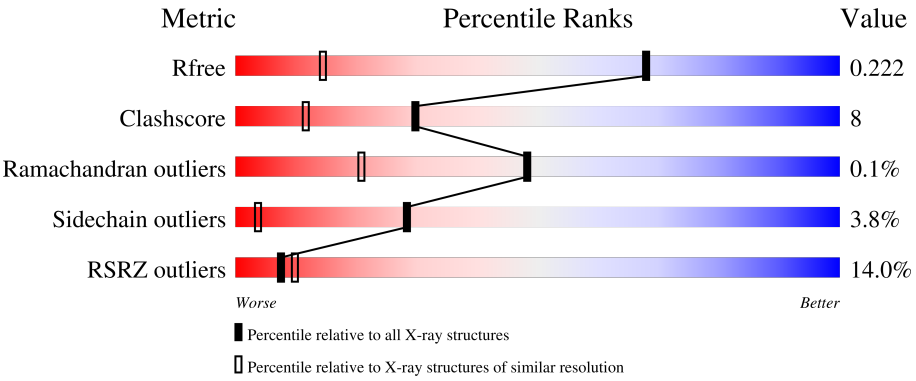
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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}	164625	1089 (1.36-1.36)
Clashscore	180529	1157 (1.36-1.36)
Ramachandran outliers	177936	1146 (1.36-1.36)
Sidechain outliers	177891	1146 (1.36-1.36)
RSRZ outliers	164620	1088 (1.36-1.36)

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 <=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	13% 73% 18% • 5%
1	B	496	14% 72% 18% • 6%

2 Entry composition (i)

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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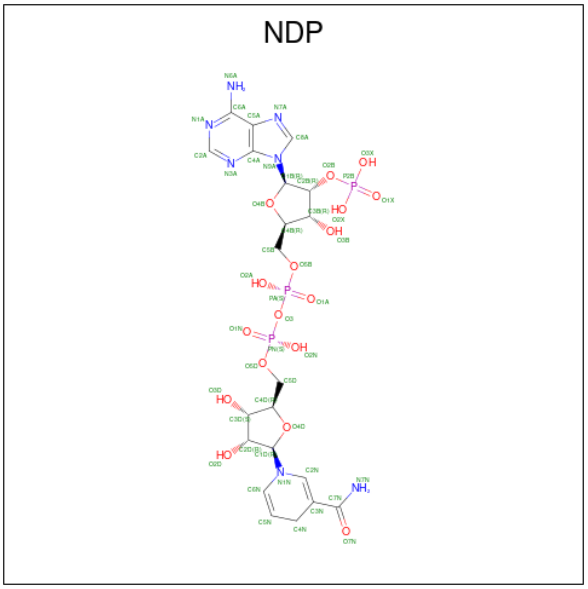
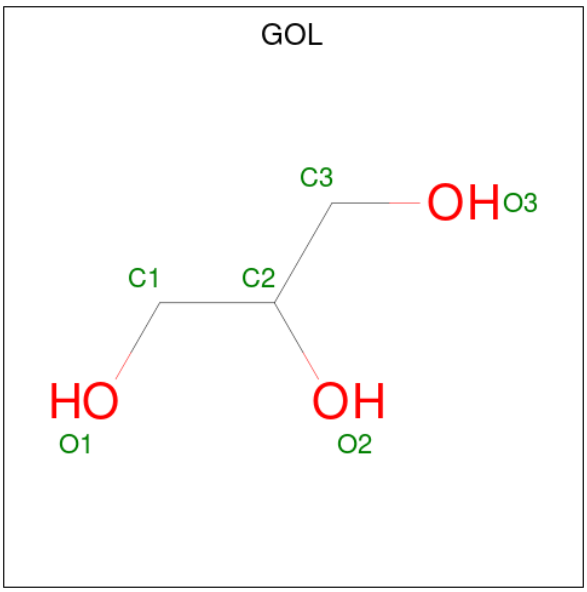
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP Q93NW7
B	-15	HIS	-	expression tag	UNP Q93NW7
B	-14	HIS	-	expression tag	UNP Q93NW7
B	-13	HIS	-	expression tag	UNP Q93NW7
B	-12	HIS	-	expression tag	UNP Q93NW7
B	-11	HIS	-	expression tag	UNP Q93NW7
B	-10	SER	-	expression tag	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 (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

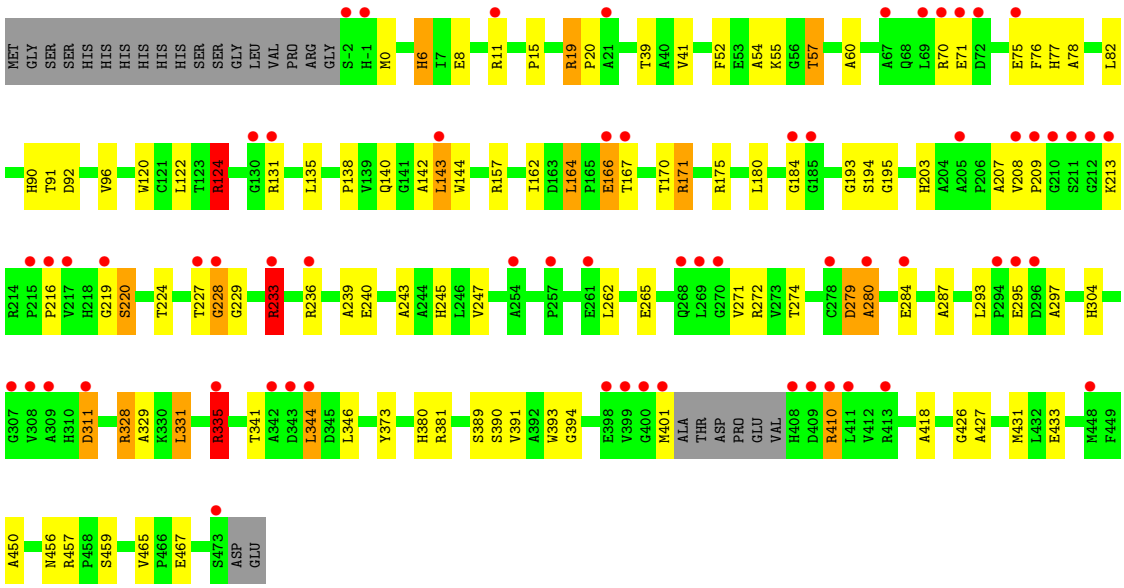
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	227	Total O 227 227	0	0
4	B	247	Total O 247 247	0	0

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.

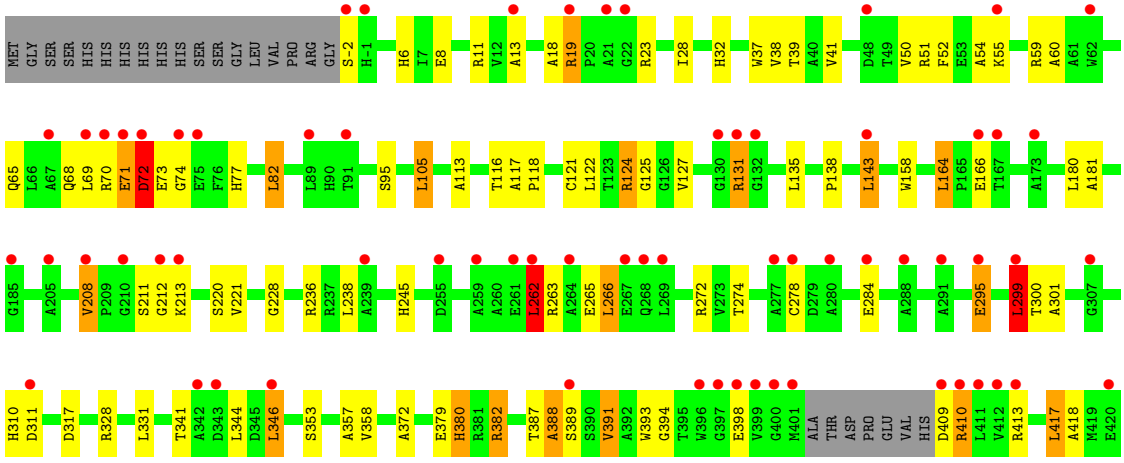
- Molecule 1: AmphB

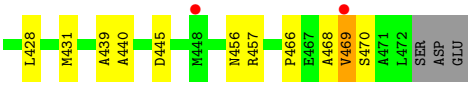
Chain A:



- Molecule 1: AmphB

Chain B:




L428
M431
A439
A440
D445
M448
N456
R457
P466
E467
A468
V469
S470
A471
L472
SER
ASP
GLU

4 Data and refinement statistics (i)

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 62.76 – 1.36	Depositor EDS
% Data completeness (in resolution range)	93.3 (62.76-1.36) 93.3 (62.76-1.36)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.56 (at 1.36Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.202 , 0.225 0.200 , 0.222	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)	0.41 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.90	61/3490 (1.7%)	1.62	36/4764 (0.8%)
1	B	1.88	51/3473 (1.5%)	1.59	36/4741 (0.8%)
All	All	1.89	112/6963 (1.6%)	1.60	72/9505 (0.8%)

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 (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	GLU	C-O	12.60	1.39	1.24
1	B	39	THR	CB-OG1	-10.11	1.27	1.43
1	A	228	GLY	C-O	-9.77	1.14	1.24
1	A	166	GLU	CB-CG	-9.61	1.23	1.52
1	B	105	LEU	CG-CD1	-9.18	1.22	1.52
1	A	389	SER	CA-CB	-8.88	1.37	1.54
1	A	207	ALA	C-O	-8.35	1.14	1.23
1	B	39	THR	CB-CG2	-8.32	1.25	1.52
1	A	166	GLU	CG-CD	-7.93	1.32	1.52
1	A	233	ARG	C-O	-7.86	1.14	1.24
1	A	54	ALA	CA-CB	7.80	1.62	1.52
1	B	54	ALA	CA-CB	7.67	1.62	1.52
1	A	287	ALA	C-O	-7.65	1.15	1.24
1	B	124	ARG	NE-CZ	7.53	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	TRP	N-CA	-7.53	1.37	1.46
1	A	96	VAL	CA-CB	-7.51	1.46	1.53
1	B	440	ALA	C-O	7.22	1.32	1.24
1	A	6	HIS	CA-CB	-7.10	1.40	1.54
1	B	417	LEU	CA-C	-7.08	1.43	1.53
1	B	284	GLU	CB-CG	-7.01	1.31	1.52
1	B	55	LYS	CB-CG	-6.96	1.31	1.52
1	A	465	VAL	CA-CB	6.93	1.60	1.53
1	A	143	LEU	N-CA	-6.93	1.37	1.46
1	B	143	LEU	CG-CD1	-6.93	1.29	1.52
1	A	60	ALA	CA-CB	-6.92	1.42	1.53
1	B	469	VAL	CB-CG2	-6.88	1.29	1.52
1	B	113	ALA	CA-CB	6.88	1.66	1.53
1	B	317	ASP	CG-OD2	-6.79	1.12	1.25
1	A	15	PRO	CG-CD	6.59	1.73	1.50
1	A	170	THR	CA-C	6.57	1.61	1.52
1	A	220	SER	N-CA	6.56	1.53	1.46
1	B	439	ALA	CA-C	-6.55	1.44	1.52
1	B	278	CYS	CA-CB	6.55	1.61	1.52
1	A	76	PHE	N-CA	6.52	1.54	1.45
1	A	96	VAL	N-CA	6.52	1.51	1.46
1	A	287	ALA	CA-CB	6.51	1.63	1.53
1	A	167	THR	C-N	6.51	1.39	1.33
1	A	450	ALA	N-CA	-6.46	1.40	1.46
1	B	116	THR	CB-OG1	-6.43	1.33	1.43
1	A	240	GLU	N-CA	6.39	1.54	1.46
1	B	28	ILE	C-O	6.37	1.30	1.24
1	B	358	VAL	CA-CB	-6.36	1.46	1.54
1	A	142	ALA	CA-CB	6.34	1.63	1.53
1	A	143	LEU	CG-CD2	-6.34	1.31	1.52
1	A	91	THR	CB-CG2	-6.33	1.31	1.52
1	B	228	GLY	C-O	-6.31	1.15	1.23
1	A	381	ARG	CB-CG	-6.27	1.33	1.52
1	B	262	LEU	CG-CD2	-6.27	1.31	1.52
1	A	279	ASP	N-CA	6.24	1.54	1.46
1	A	280	ALA	CA-C	6.24	1.61	1.52
1	B	418	ALA	CA-CB	6.24	1.63	1.53
1	B	278	CYS	N-CA	6.21	1.54	1.46
1	A	456	ASN	CA-C	-6.20	1.44	1.52
1	A	331	LEU	N-CA	-6.16	1.39	1.46
1	A	284	GLU	CB-CG	-6.04	1.34	1.52
1	B	272	ARG	CZ-NH2	-5.95	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	LEU	CA-C	-5.95	1.45	1.53
1	B	124	ARG	CZ-NH2	-5.94	1.25	1.33
1	B	389	SER	N-CA	5.92	1.53	1.46
1	A	389	SER	CB-OG	-5.85	1.30	1.42
1	A	328	ARG	CZ-NH2	-5.84	1.25	1.33
1	A	78	ALA	CA-C	-5.80	1.45	1.52
1	A	82	LEU	CG-CD2	-5.78	1.33	1.52
1	B	117	ALA	N-CA	5.75	1.53	1.45
1	B	379	GLU	CD-OE1	-5.74	1.14	1.25
1	A	19	ARG	CZ-NH1	-5.74	1.24	1.32
1	A	335	ARG	CB-CG	-5.63	1.35	1.52
1	B	372	ALA	N-CA	-5.61	1.39	1.46
1	B	52	PHE	CG-CD1	-5.61	1.27	1.38
1	A	459	SER	C-O	5.55	1.30	1.24
1	A	6	HIS	CB-CG	-5.50	1.42	1.50
1	B	158	TRP	CA-C	-5.45	1.46	1.52
1	B	127	VAL	N-CA	5.44	1.52	1.46
1	A	389	SER	C-O	5.44	1.30	1.23
1	B	69	LEU	N-CA	-5.43	1.39	1.46
1	B	18	ALA	N-CA	5.43	1.53	1.46
1	B	295	GLU	N-CA	5.42	1.53	1.46
1	B	38	VAL	N-CA	5.40	1.52	1.46
1	B	95	SER	C-N	-5.38	1.28	1.33
1	B	143	LEU	CB-CG	-5.36	1.42	1.53
1	A	52	PHE	CG-CD2	-5.34	1.27	1.38
1	B	164	LEU	CG-CD1	-5.34	1.34	1.52
1	A	418	ALA	CA-CB	5.33	1.61	1.53
1	A	427	ALA	CA-CB	-5.33	1.44	1.53
1	B	389	SER	C-O	5.33	1.30	1.23
1	A	162	ILE	N-CA	5.32	1.52	1.46
1	B	456	ASN	CA-C	-5.31	1.45	1.52
1	A	164	LEU	CG-CD1	-5.30	1.35	1.52
1	A	272	ARG	CZ-NH2	-5.29	1.26	1.33
1	B	143	LEU	N-CA	-5.28	1.39	1.46
1	A	410	ARG	CZ-NH1	5.24	1.40	1.32
1	A	344	LEU	CG-CD1	-5.23	1.35	1.52
1	B	388	ALA	CA-C	-5.20	1.45	1.52
1	A	120	TRP	C-O	5.20	1.30	1.24
1	B	138	PRO	N-CA	-5.18	1.40	1.47
1	B	60	ALA	CA-CB	-5.18	1.45	1.53
1	A	39	THR	CA-CB	5.18	1.61	1.53
1	A	328	ARG	NE-CZ	-5.18	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	CYS	C-O	5.18	1.30	1.24
1	A	247	VAL	CA-CB	-5.16	1.47	1.53
1	B	331	LEU	N-CA	-5.14	1.40	1.46
1	A	124	ARG	NE-CZ	5.13	1.38	1.33
1	B	50	VAL	C-O	5.13	1.30	1.24
1	B	181	ALA	C-O	5.12	1.30	1.24
1	A	142	ALA	CA-C	-5.12	1.45	1.52
1	A	297	ALA	CA-CB	-5.10	1.47	1.53
1	B	69	LEU	CA-CB	5.08	1.61	1.53
1	B	357	ALA	CA-C	-5.07	1.45	1.52
1	A	57	THR	CA-C	-5.04	1.46	1.53
1	A	390	SER	CB-OG	-5.03	1.32	1.42
1	A	465	VAL	C-O	-5.03	1.18	1.24
1	A	193	GLY	N-CA	5.01	1.52	1.45

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	382	ARG	CD-NE-CZ	16.52	147.53	124.40
1	B	382	ARG	CB-CG-CD	12.75	140.63	111.30
1	B	72	ASP	CB-CA-C	-11.65	96.37	111.40
1	A	167	THR	CB-CA-C	11.17	128.70	110.16
1	A	55	LYS	CD-CE-NZ	-10.71	77.61	111.90
1	B	382	ARG	NE-CZ-NH2	-10.51	109.74	119.20
1	A	293	LEU	CA-C-N	9.99	130.10	120.31
1	A	293	LEU	C-N-CA	9.99	130.10	120.31
1	A	19	ARG	NE-CZ-NH2	9.79	128.01	119.20
1	A	328	ARG	NE-CZ-NH2	-9.63	110.53	119.20
1	A	166	GLU	CB-CG-CD	-9.14	97.06	112.60
1	B	71	GLU	N-CA-C	-9.10	100.93	111.03
1	A	166	GLU	CA-C-N	-8.94	110.39	123.00
1	A	166	GLU	C-N-CA	-8.94	110.39	123.00
1	B	382	ARG	NE-CZ-NH1	8.93	130.43	121.50
1	A	284	GLU	CB-CG-CD	-8.68	97.85	112.60
1	B	124	ARG	NE-CZ-NH2	8.65	126.98	119.20
1	B	166	GLU	O-C-N	7.40	130.88	122.22
1	B	19	ARG	NE-CZ-NH2	7.34	125.80	119.20
1	A	335	ARG	CD-NE-CZ	7.20	134.48	124.40
1	B	341	THR	OG1-CB-CG2	7.15	123.60	109.30
1	A	167	THR	CA-C-N	-6.97	114.20	122.22
1	A	167	THR	C-N-CA	-6.97	114.20	122.22
1	B	82	LEU	CB-CG-CD1	6.67	130.72	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	457	ARG	N-CA-CB	6.53	119.84	110.77
1	B	74	GLY	N-CA-C	-6.46	98.87	112.45
1	A	243	ALA	CA-C-O	-6.38	114.13	121.15
1	A	227	THR	O-C-N	-6.37	114.11	122.59
1	B	212	GLY	CA-C-N	-6.27	111.66	122.14
1	B	212	GLY	C-N-CA	-6.27	111.66	122.14
1	A	175	ARG	NE-CZ-NH2	-6.25	113.57	119.20
1	A	457	ARG	N-CA-CB	6.19	119.37	110.77
1	A	328	ARG	NE-CZ-NH1	6.18	127.69	121.50
1	A	124	ARG	NE-CZ-NH2	6.16	124.74	119.20
1	B	166	GLU	CA-C-N	-6.11	114.38	123.00
1	B	166	GLU	C-N-CA	-6.11	114.38	123.00
1	B	70	ARG	CA-C-N	5.98	128.76	120.63
1	B	70	ARG	C-N-CA	5.98	128.76	120.63
1	A	240	GLU	CG-CD-OE1	5.96	132.11	118.40
1	B	389	SER	O-C-N	-5.95	116.14	123.33
1	B	299	LEU	CD1-CG-CD2	-5.94	97.73	110.80
1	A	71	GLU	N-CA-C	-5.93	104.73	111.14
1	A	166	GLU	N-CA-CB	5.92	119.45	110.28
1	A	122	LEU	CB-CG-CD2	5.90	128.41	110.70
1	A	239	ALA	O-C-N	5.76	128.23	122.12
1	B	124	ARG	CD-NE-CZ	-5.65	116.49	124.40
1	A	295	GLU	O-C-N	5.63	127.94	122.09
1	B	122	LEU	CB-CG-CD2	5.61	127.53	110.70
1	B	346	LEU	CB-CG-CD1	5.48	127.13	110.70
1	A	228	GLY	N-CA-C	-5.45	102.64	110.60
1	A	15	PRO	N-CD-CG	-5.43	95.05	103.20
1	A	271	VAL	N-CA-C	5.43	116.09	109.30
1	A	39	THR	CA-CB-OG1	-5.42	101.47	109.60
1	A	311	ASP	CB-CG-OD1	5.40	130.83	118.40
1	A	184	GLY	CA-C-O	-5.39	112.85	119.69
1	A	157	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	B	263	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	B	124	ARG	NH1-CZ-NH2	-5.29	112.42	119.30
1	B	278	CYS	N-CA-C	-5.25	98.46	107.23
1	A	433	GLU	CB-CG-CD	5.21	121.47	112.60
1	B	263	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	167	THR	CA-CB-CG2	5.21	119.36	110.50
1	B	398	GLU	N-CA-C	5.18	121.84	110.80
1	B	143	LEU	CB-CG-CD2	5.18	126.23	110.70
1	A	219	GLY	O-C-N	5.17	128.13	122.60
1	B	328	ARG	NE-CZ-NH2	-5.17	114.55	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	51	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A	216	PRO	CA-C-O	-5.08	115.54	121.34
1	B	391	VAL	CG1-CB-CG2	5.04	121.89	110.80
1	B	65	GLN	CA-C-O	5.03	125.75	120.42
1	B	380	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	B	468	ALA	CA-C-O	-5.01	114.68	120.24

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	GLY	Peptide,Mainchain
1	A	280	ALA	Mainchain
1	B	72	ASP	Peptide

5.2 Too-close contacts (i)

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	53	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
4	A	227	0	0	5	0
4	B	247	0	0	12	0
All	All	7404	0	6822	116	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 (116) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH21	1:A:11:ARG:HG3	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:HG3	1:A:11:ARG:NH2	1.90	0.77
1:A:335:ARG:HH21	1:A:335:ARG:CB	1.97	0.77
1:A:166:GLU:OE2	1:A:166:GLU:N	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:HH21	1:A:335:ARG:HB3	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
1:A:11:ARG:HH21	1:A:11:ARG:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:A:70:ARG:NH2	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:B:299:LEU:HD23	1:B:299:LEU:C	2.27	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:HH21	1:A:335:ARG:HB2	1.71	0.54
1:A:131:ARG:HH21	1:B:131:ARG:NH1	2.00	0.54
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:A:166:GLU:N	1:A:166:GLU:CD	2.66	0.53
1:B:77:HIS:HE1	1:B:180:LEU:O	1.91	0.53
1:A:166:GLU:CD	1:A:166:GLU:H	2.15	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:A:236:ARG:HD3	1:A:265:GLU:CD	2.36	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
1:B:310:HIS:HD2	1:B:311:ASP:OD2	1.96	0.48
1:B:299:LEU:C	1:B:299:LEU:CD2	2.86	0.48
1:B:6:HIS:CE1	1:B:8:GLU:OE1	2.68	0.47
1:B:59:ARG:HB2	1:B:105:LEU:HD12	1.95	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:353:SER:O	2:B:476:NDP:H6N	2.15	0.47
1:B:391:VAL:HG22	1:B:431:MET:SD	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:A:331:LEU:C	1:A:331:LEU:HD23	2.43	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:A:279:ASP:CG	1:A:328:ARG:HH22	2.26	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
1:B:413:ARG:HH11	1:B:413:ARG:CG	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%)	44 19
1	B	464/496 (94%)	452 (97%)	12 (3%)	0	100 100
All	All	930/992 (94%)	906 (97%)	23 (2%)	1 (0%)	48 21

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%)	318 (97%)	11 (3%)	33 6
1	B	327/351 (93%)	313 (96%)	14 (4%)	25 3
All	All	656/702 (93%)	631 (96%)	25 (4%)	28 4

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	GLU
1	A	124	ARG
1	A	143	LEU
1	A	171	ARG
1	A	213	LYS

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Mol	Chain	Res	Type
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	23	ARG
1	B	82	LEU
1	B	124	ARG
1	B	131	ARG
1	B	143	LEU
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	409	ASP
1	B	410	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
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	310	HIS
1	A	336	HIS
1	A	380	HIS
1	A	423	HIS
1	B	6	HIS
1	B	32	HIS
1	B	65	GLN
1	B	68	GLN
1	B	77	HIS

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Mol	Chain	Res	Type
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 oligosaccharides 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	-	47,52,52	2.11	14 (29%)	61,80,80	1.93	14 (22%)
3	GOL	B	477	-	5,5,5	0.98	0	5,5,5	0.56	0
2	NDP	B	476	-	47,52,52	1.57	10 (21%)	61,80,80	2.02	15 (24%)

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	-	-	6/30/77/77	0/5/5/5
3	GOL	B	477	-	-	0/4/4/4	-
2	NDP	B	476	-	-	7/30/77/77	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	476	NDP	PA-O3	6.45	1.66	1.59
2	B	476	NDP	O4B-C1B	5.10	1.47	1.40
2	A	476	NDP	C4N-C3N	-5.03	1.40	1.50
2	A	476	NDP	P2B-O2B	3.89	1.66	1.59
2	A	476	NDP	C4A-N3A	3.54	1.40	1.35
2	A	476	NDP	PN-O3	3.52	1.63	1.59
2	A	476	NDP	C2A-N1A	3.47	1.40	1.33
2	B	476	NDP	C2A-N3A	3.20	1.37	1.32
2	B	476	NDP	C4N-C3N	-3.18	1.44	1.50
2	A	476	NDP	C4N-C5N	-3.09	1.41	1.49
2	A	476	NDP	O4B-C1B	2.93	1.44	1.40
2	B	476	NDP	C4A-N3A	2.90	1.39	1.35
2	B	476	NDP	P2B-O2B	2.88	1.64	1.59
2	A	476	NDP	C2A-N3A	2.79	1.36	1.32
2	A	476	NDP	C2N-C3N	2.71	1.42	1.35
2	B	476	NDP	C4N-C5N	-2.59	1.42	1.49
2	B	476	NDP	C3B-C4B	-2.39	1.46	1.53
2	B	476	NDP	C2A-N1A	2.30	1.38	1.33
2	A	476	NDP	PN-O2N	-2.21	1.45	1.55
2	A	476	NDP	C1D-N1N	2.16	1.52	1.46
2	A	476	NDP	C7N-C3N	2.16	1.53	1.48
2	A	476	NDP	C3B-C4B	-2.14	1.47	1.53
2	B	476	NDP	O4D-C1D	2.03	1.46	1.42
2	B	476	NDP	C6N-C5N	2.01	1.39	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	476	NDP	C4B-O4B-C1B	-7.22	103.32	109.92
2	A	476	NDP	N3A-C2A-N1A	-6.30	120.12	128.67
2	B	476	NDP	N3A-C2A-N1A	-5.27	121.52	128.67
2	B	476	NDP	O4B-C4B-C3B	5.02	115.12	105.15
2	A	476	NDP	O4B-C1B-C2B	-4.82	98.38	106.61
2	A	476	NDP	O4B-C1B-N9A	-4.34	102.99	108.75
2	B	476	NDP	C6N-N1N-C2N	4.16	123.77	119.32
2	A	476	NDP	C1B-N9A-C4A	-3.83	119.91	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	476	NDP	C4A-C5A-N7A	-3.68	105.45	109.34
2	A	476	NDP	C6N-N1N-C2N	3.58	123.15	119.32
2	A	476	NDP	O4B-C4B-C3B	3.57	112.23	105.15
2	B	476	NDP	O7N-C7N-C3N	-3.52	114.27	120.90
2	B	476	NDP	O4D-C4D-C3D	3.45	112.00	105.15
2	A	476	NDP	C1D-N1N-C6N	-3.29	113.81	120.77
2	A	476	NDP	C2D-C3D-C4D	3.12	108.63	102.61
2	B	476	NDP	C1D-N1N-C6N	-2.96	114.51	120.77
2	A	476	NDP	C4A-C5A-N7A	-2.73	106.45	109.34
2	A	476	NDP	C2B-C3B-C4B	-2.66	96.28	101.99
2	B	476	NDP	N6A-C6A-N1A	2.54	123.77	118.33
2	A	476	NDP	O2X-P2B-O1X	2.43	120.28	110.83
2	B	476	NDP	O2B-P2B-O1X	-2.42	100.70	109.33
2	B	476	NDP	C3N-C2N-N1N	-2.35	119.75	123.20
2	A	476	NDP	C5B-C4B-C3B	2.25	123.31	115.21
2	A	476	NDP	O2B-P2B-O1X	-2.24	101.35	109.33
2	B	476	NDP	O3-PN-O1N	-2.23	104.01	110.70
2	B	476	NDP	C3N-C7N-N7N	2.23	121.62	117.67
2	B	476	NDP	O3B-C3B-C4B	-2.19	104.79	111.08
2	A	476	NDP	C4B-O4B-C1B	-2.12	107.98	109.92
2	B	476	NDP	C5A-C6A-N1A	-2.12	115.17	120.23

There are no chirality outliers.

All (13) torsion outliers are listed below:

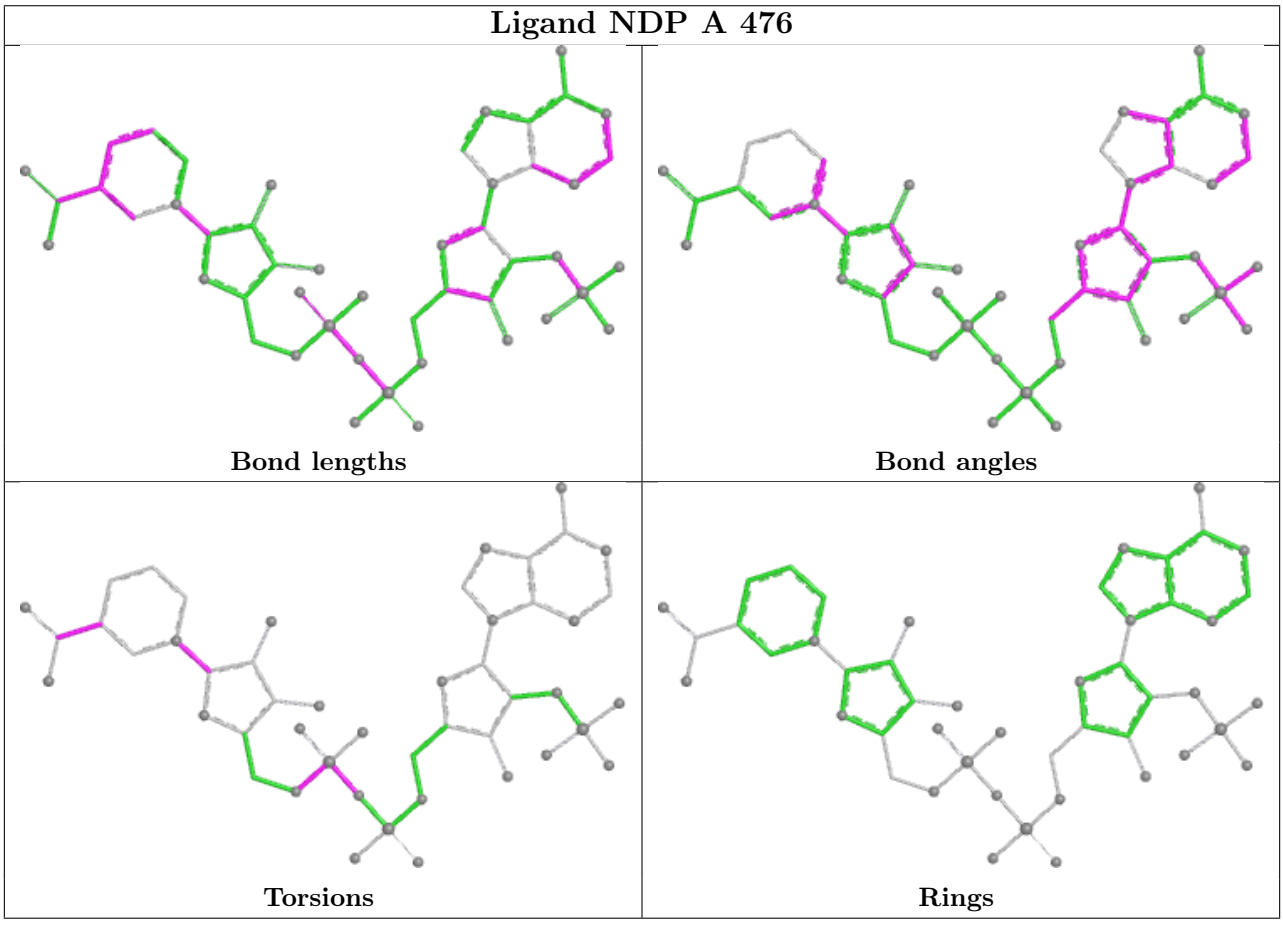
Mol	Chain	Res	Type	Atoms
2	A	476	NDP	C5D-O5D-PN-O3
2	A	476	NDP	C5D-O5D-PN-O1N
2	A	476	NDP	C5D-O5D-PN-O2N
2	B	476	NDP	C5D-O5D-PN-O3
2	B	476	NDP	C5D-O5D-PN-O2N
2	A	476	NDP	O4D-C1D-N1N-C6N
2	B	476	NDP	O4D-C1D-N1N-C6N
2	B	476	NDP	C5D-O5D-PN-O1N
2	A	476	NDP	C2N-C3N-C7N-N7N
2	B	476	NDP	C2N-C3N-C7N-N7N
2	A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

There are no ring outliers.

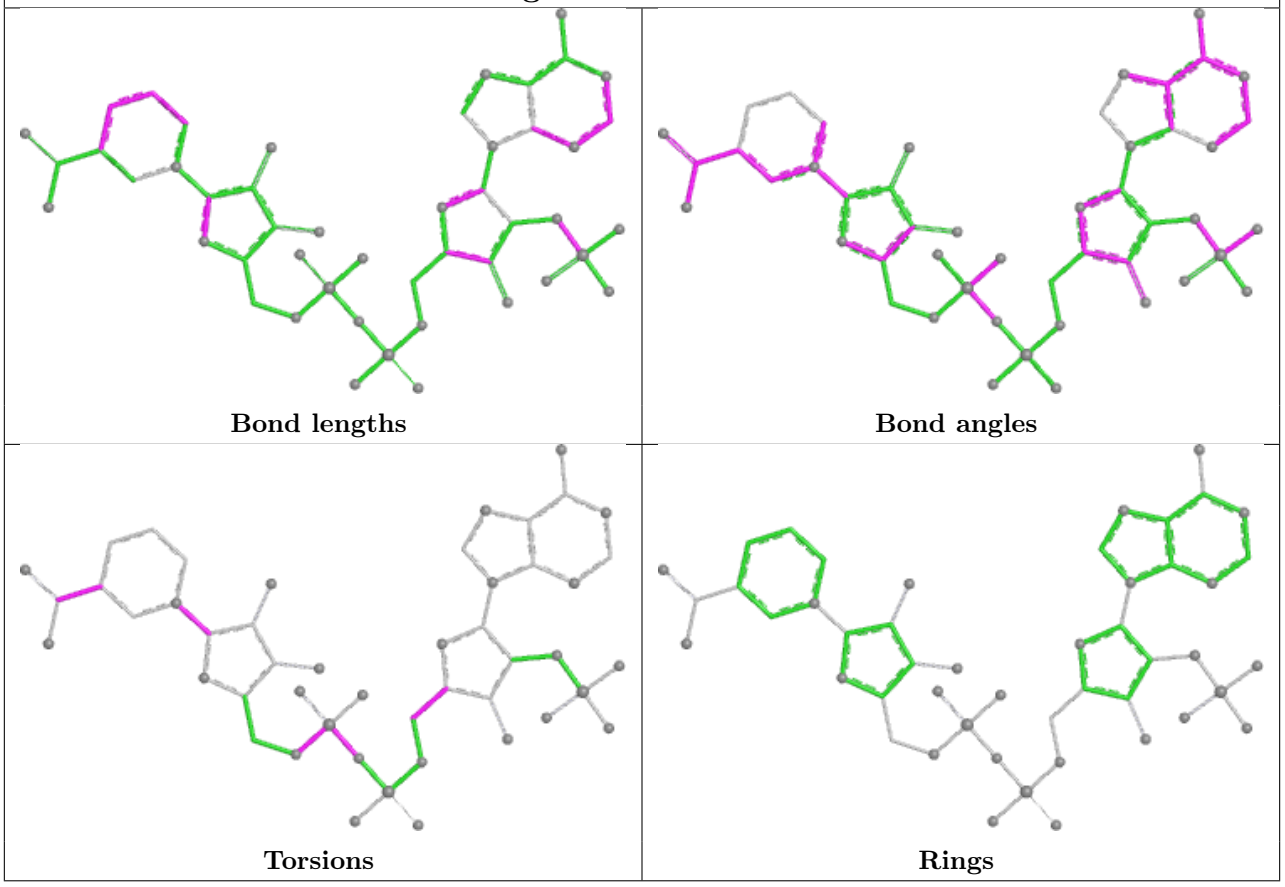
2 monomers are involved in 14 short contacts:

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 then 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.



Ligand NDP B 476



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^{th} 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%)	0.86	63 (13%)	8	10	7, 14, 28, 42	0
1	B	468/496 (94%)	0.83	68 (14%)	7	9	6, 13, 28, 42	0
All	All	938/992 (94%)	0.85	131 (13%)	7	10	6, 14, 28, 42	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	399	VAL	6.2
1	A	213	LYS	5.9
1	B	278	CYS	5.9
1	B	401	MET	5.9
1	A	401	MET	5.7
1	B	411	LEU	5.5
1	A	208	VAL	5.4
1	A	410	ARG	5.3
1	B	72	ASP	5.0
1	B	410	ARG	4.8
1	B	21	ALA	4.8
1	A	411	LEU	4.7
1	A	-1	HIS	4.6
1	B	213	LYS	4.4
1	A	209	PRO	4.3
1	A	210	GLY	4.3
1	A	413	ARG	4.3
1	B	399	VAL	4.3
1	A	11	ARG	4.2
1	A	278	CYS	4.1
1	A	131	ARG	4.1
1	A	295	GLU	4.1
1	A	408	HIS	4.0
1	B	131	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	75	GLU	3.9
1	B	74	GLY	3.9
1	A	294	PRO	3.9
1	A	261	GLU	3.7
1	B	400	GLY	3.7
1	A	308	VAL	3.6
1	B	143	LEU	3.5
1	A	211	SER	3.5
1	B	166	GLU	3.5
1	B	295	GLU	3.5
1	B	19	ARG	3.5
1	B	413	ARG	3.5
1	A	212	GLY	3.4
1	A	311	ASP	3.4
1	B	343	ASP	3.4
1	A	166	GLU	3.2
1	B	-1	HIS	3.2
1	A	307	GLY	3.1
1	B	261	GLU	3.1
1	B	396	TRP	3.1
1	A	269	LEU	3.1
1	B	264	ALA	3.1
1	A	-2	SER	3.1
1	A	217	VAL	3.0
1	A	72	ASP	3.0
1	B	130	GLY	3.0
1	B	284	GLU	3.0
1	A	280	ALA	3.0
1	B	69	LEU	3.0
1	B	75	GLU	2.9
1	A	167	THR	2.9
1	A	257	PRO	2.9
1	B	210	GLY	2.9
1	B	280	ALA	2.9
1	B	291	ALA	2.9
1	B	412	VAL	2.8
1	A	400	GLY	2.8
1	A	215	PRO	2.8
1	B	-2	SER	2.8
1	B	262	LEU	2.8
1	A	71	GLU	2.8
1	B	389	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	236	ARG	2.7
1	A	398	GLU	2.7
1	B	91	THR	2.6
1	B	409	ASP	2.6
1	B	89	LEU	2.6
1	B	397	GLY	2.6
1	A	335	ARG	2.5
1	B	67	ALA	2.5
1	A	143	LEU	2.5
1	B	299	LEU	2.5
1	A	184	GLY	2.5
1	B	469	VAL	2.5
1	B	420	GLU	2.5
1	A	296	ASP	2.5
1	B	62	TRP	2.5
1	A	67	ALA	2.5
1	B	13	ALA	2.5
1	B	167	THR	2.5
1	B	205	ALA	2.5
1	A	344	LEU	2.5
1	A	216	PRO	2.5
1	B	267	GLU	2.5
1	A	185	GLY	2.4
1	A	473	SER	2.4
1	B	70	ARG	2.4
1	A	21	ALA	2.4
1	B	71	GLU	2.4
1	A	233	ARG	2.4
1	A	284	GLU	2.4
1	A	342	ALA	2.4
1	B	48	ASP	2.4
1	B	239	ALA	2.4
1	B	268	GLN	2.4
1	A	343	ASP	2.4
1	A	205	ALA	2.4
1	A	254	ALA	2.3
1	B	259	ALA	2.3
1	B	342	ALA	2.3
1	A	130	GLY	2.3
1	B	22	GLY	2.3
1	A	69	LEU	2.3
1	A	70	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	212	GLY	2.3
1	B	346	LEU	2.3
1	A	228	GLY	2.3
1	A	309	ALA	2.3
1	B	173	ALA	2.3
1	B	208	VAL	2.3
1	B	269	LEU	2.2
1	B	307	GLY	2.2
1	B	288	ALA	2.2
1	B	255	ASP	2.2
1	A	268	GLN	2.2
1	A	227	THR	2.2
1	B	398	GLU	2.1
1	B	448	MET	2.1
1	A	219	GLY	2.1
1	A	270	GLY	2.1
1	B	311	ASP	2.1
1	B	55	LYS	2.1
1	A	409	ASP	2.1
1	B	185	GLY	2.1
1	B	132	GLY	2.0
1	A	448	MET	2.0
1	B	277	ALA	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^{th} 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.

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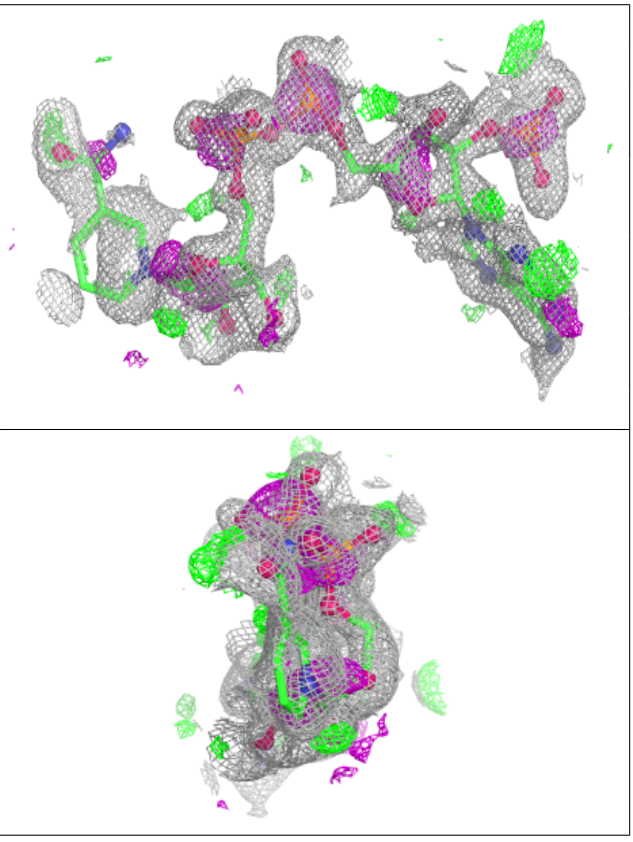
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

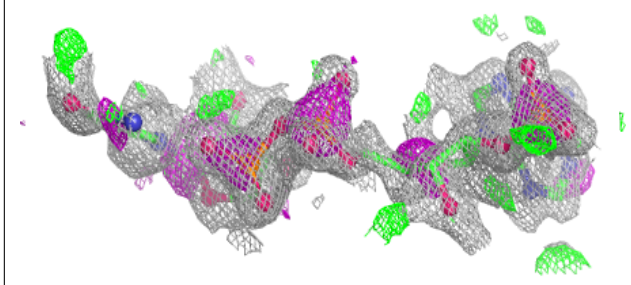
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NDP	A	476	48/48	0.90	0.12	18,23,36,38	0
3	GOL	B	477	6/6	0.92	0.08	15,17,18,18	0
2	NDP	B	476	48/48	0.93	0.10	14,19,23,27	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NDP A 476:

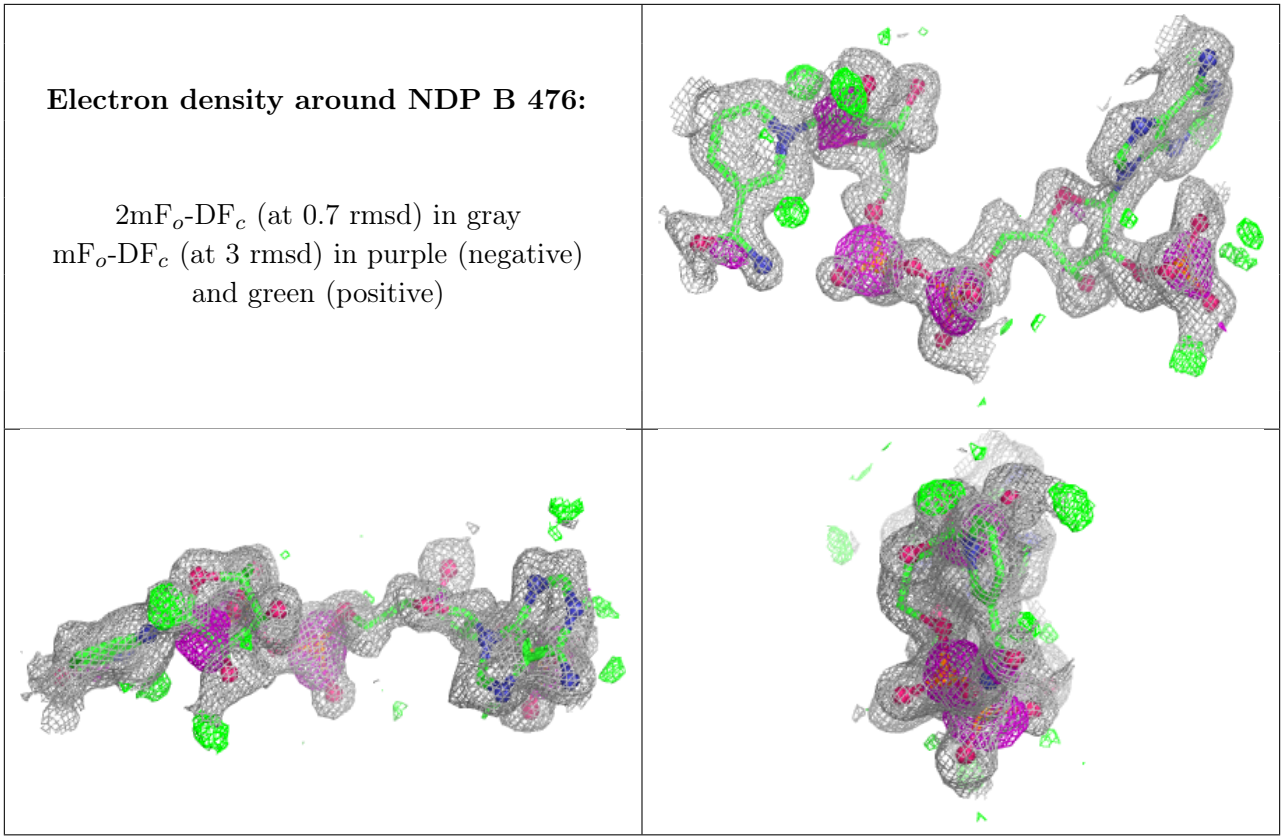
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around NDP B 476:

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



6.5 Other polymers (i)

There are no such residues in this entry.