



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 08:02 PM BST

PDB ID : 3MJS
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 : 1.40 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 : 2.13.1
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) : 2.13.1

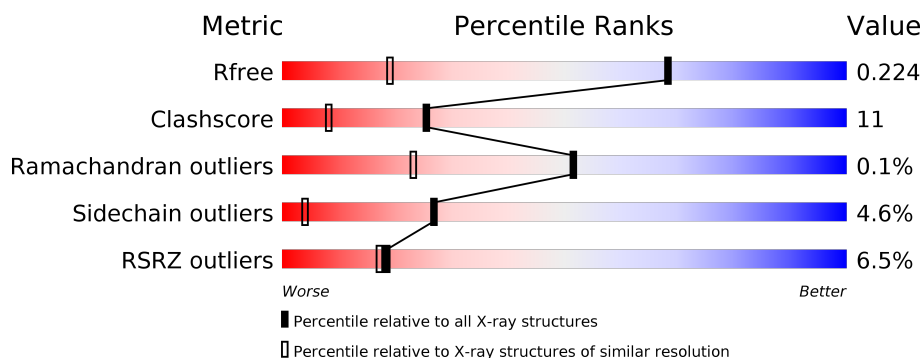
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	 7% 73% 20% . . .
1	B	496	 6% 74% 17% 5% .

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
4	MLT	B	478	-	-	X	-
5	GOL	A	479	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7572 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
			3465	2163	635	658	9			
1	B	475	Total	C	N	O	S	0	0	0
			3459	2160	634	656	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

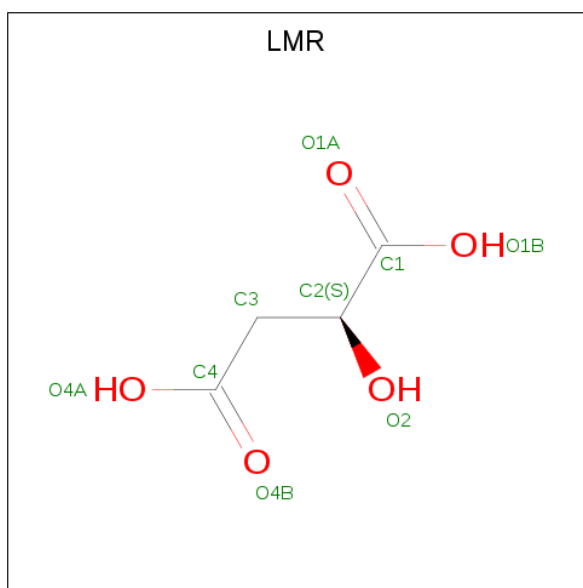
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	EXPRESSION TAG	UNP Q93NW7
B	-15	HIS	-	EXPRESSION TAG	UNP Q93NW7
B	-14	HIS	-	EXPRESSION TAG	UNP Q93NW7
B	-13	HIS	-	EXPRESSION TAG	UNP Q93NW7
B	-12	HIS	-	EXPRESSION TAG	UNP Q93NW7
B	-11	HIS	-	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

- # NDP

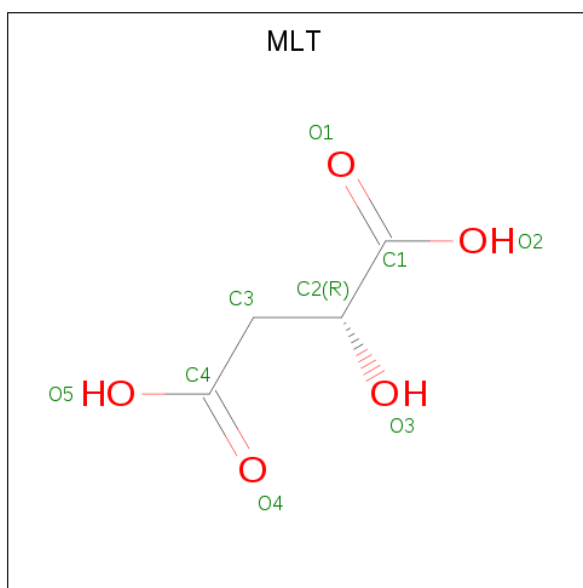
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula: C₄H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 4 is D-MALATE (three-letter code: MLT) (formula: C₄H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	4	5		
4	B	1	Total	C	O	0	0
			9	4	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			9	4	5		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	248	Total	O	0	0
			248	248		
6	B	256	Total	O	0	0
			256	256		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.44Å 63.71Å 71.82Å 72.77° 67.09° 89.79°	Depositor
Resolution (Å)	62.68 – 1.40 43.98 – 1.40	Depositor EDS
% Data completeness (in resolution range)	94.8 (62.68-1.40) 94.8 (43.98-1.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.199 , 0.226 0.198 , 0.224	Depositor DCC
R_{free} test set	8865 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.083 for h,-k,h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7572	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 5.72% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LMR, MLT, 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	1.51	36/3535 (1.0%)	1.49	53/4829 (1.1%)
1	B	1.51	37/3529 (1.0%)	1.51	60/4821 (1.2%)
All	All	1.51	73/7064 (1.0%)	1.50	113/9650 (1.2%)

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	GLU	CG-CD	-12.58	1.33	1.51
1	A	389	SER	CB-OG	-11.61	1.27	1.42
1	B	69	LEU	C-N	10.08	1.57	1.34
1	B	457	ARG	CB-CG	-9.57	1.26	1.52
1	B	166	GLU	CG-CD	-9.39	1.37	1.51
1	A	8	GLU	CD-OE1	-9.09	1.15	1.25
1	B	284	GLU	CB-CG	-9.06	1.34	1.52
1	B	8	GLU	CD-OE2	-8.88	1.15	1.25
1	B	469	VAL	CB-CG2	-8.87	1.34	1.52
1	A	236	ARG	CB-CG	-8.40	1.29	1.52
1	A	284	GLU	CB-CG	-8.32	1.36	1.52
1	B	76	PHE	CE1-CZ	-8.12	1.22	1.37
1	B	87	GLU	CD-OE2	-7.60	1.17	1.25
1	A	447	GLU	CD-OE2	-7.20	1.17	1.25
1	A	389	SER	CA-CB	-7.14	1.42	1.52
1	A	272	ARG	CZ-NH1	-6.99	1.24	1.33
1	A	166	GLU	CB-CG	-6.93	1.39	1.52
1	B	158	TRP	CZ3-CH2	6.92	1.51	1.40
1	A	153	GLU	CD-OE1	-6.81	1.18	1.25
1	A	379	GLU	CG-CD	6.72	1.62	1.51
1	A	278	CYS	CB-SG	-6.72	1.70	1.82
1	B	166	GLU	C-O	6.69	1.36	1.23
1	A	71	GLU	CG-CD	-6.68	1.42	1.51
1	A	73	GLU	CD-OE2	-6.65	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ARG	CZ-NH1	-6.58	1.24	1.33
1	B	153	GLU	CD-OE1	-6.51	1.18	1.25
1	B	95	SER	CB-OG	6.47	1.50	1.42
1	B	55	LYS	CB-CG	-6.46	1.35	1.52
1	A	208	VAL	C-O	6.37	1.35	1.23
1	A	394	GLY	C-O	6.34	1.33	1.23
1	A	272	ARG	CZ-NH2	-6.32	1.24	1.33
1	B	208	VAL	CB-CG1	-6.18	1.39	1.52
1	B	-2	SER	CB-OG	6.18	1.50	1.42
1	B	379	GLU	CD-OE1	-6.10	1.19	1.25
1	B	389	SER	CB-OG	6.04	1.50	1.42
1	B	339	GLU	CB-CG	6.00	1.63	1.52
1	A	433	GLU	CG-CD	6.00	1.60	1.51
1	A	339	GLU	CD-OE2	-5.99	1.19	1.25
1	B	166	GLU	CB-CG	-5.99	1.40	1.52
1	B	143	LEU	N-CA	-5.98	1.34	1.46
1	B	394	GLY	C-O	5.98	1.33	1.23
1	B	391	VAL	CB-CG1	-5.96	1.40	1.52
1	A	375	ASP	CB-CG	5.95	1.64	1.51
1	B	76	PHE	CG-CD2	-5.93	1.29	1.38
1	B	124	ARG	NE-CZ	5.88	1.40	1.33
1	A	95	SER	CB-OG	5.86	1.49	1.42
1	A	153	GLU	CG-CD	-5.83	1.43	1.51
1	A	76	PHE	CE2-CZ	-5.79	1.26	1.37
1	A	23	ARG	CB-CG	-5.76	1.36	1.52
1	A	124	ARG	CG-CD	-5.74	1.37	1.51
1	B	91	THR	CB-CG2	-5.68	1.33	1.52
1	B	94	GLY	C-N	5.63	1.47	1.34
1	B	127	VAL	CB-CG1	5.62	1.64	1.52
1	A	328	ARG	CD-NE	-5.58	1.36	1.46
1	A	344	LEU	CG-CD1	-5.57	1.31	1.51
1	A	87	GLU	CD-OE1	-5.56	1.19	1.25
1	A	19	ARG	CZ-NH1	-5.56	1.25	1.33
1	A	339	GLU	CB-CG	5.55	1.62	1.52
1	B	262	LEU	CG-CD2	-5.53	1.31	1.51
1	B	70	ARG	C-N	5.46	1.46	1.34
1	A	158	TRP	CD1-NE1	5.46	1.47	1.38
1	B	328	ARG	CD-NE	-5.43	1.37	1.46
1	B	105	LEU	CG-CD1	-5.42	1.31	1.51
1	B	284	GLU	CG-CD	-5.41	1.43	1.51
1	B	240	GLU	CD-OE1	-5.40	1.19	1.25
1	B	240	GLU	CD-OE2	-5.31	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	GLU	C-N	-5.27	1.22	1.34
1	B	339	GLU	CD-OE1	-5.26	1.19	1.25
1	B	51	ARG	CZ-NH1	-5.24	1.26	1.33
1	A	335	ARG	CB-CG	-5.22	1.38	1.52
1	A	9	TRP	CG-CD1	5.20	1.44	1.36
1	A	6	HIS	CA-CB	-5.17	1.42	1.53
1	B	250	SER	CB-OG	5.09	1.48	1.42

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	ARG	NE-CZ-NH1	-15.55	112.53	120.30
1	B	335	ARG	NE-CZ-NH2	14.76	127.68	120.30
1	A	19	ARG	NE-CZ-NH2	14.71	127.65	120.30
1	B	200	ARG	NE-CZ-NH1	14.43	127.52	120.30
1	A	335	ARG	NE-CZ-NH2	13.81	127.20	120.30
1	A	4	ARG	NE-CZ-NH1	13.25	126.93	120.30
1	B	82	LEU	CB-CG-CD1	12.39	132.07	111.00
1	A	214	ARG	NE-CZ-NH2	-12.33	114.14	120.30
1	A	335	ARG	NE-CZ-NH1	-12.18	114.21	120.30
1	B	335	ARG	NE-CZ-NH1	-12.15	114.22	120.30
1	A	328	ARG	NE-CZ-NH2	11.62	126.11	120.30
1	A	55	LYS	CD-CE-NZ	-11.60	85.01	111.70
1	A	176	LEU	CB-CG-CD1	11.52	130.58	111.00
1	B	19	ARG	NE-CZ-NH2	10.66	125.63	120.30
1	B	124	ARG	NE-CZ-NH2	10.47	125.53	120.30
1	B	55	LYS	CD-CE-NZ	-10.42	87.73	111.70
1	A	312	ASP	CB-CG-OD2	-10.41	108.93	118.30
1	B	148	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	B	4	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	A	148	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	B	148	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	A	115	LEU	CB-CG-CD1	-10.10	93.83	111.00
1	B	263	ARG	NE-CZ-NH1	-9.30	115.65	120.30
1	B	115	LEU	CB-CG-CD1	-9.19	95.37	111.00
1	B	279	ASP	CB-CG-OD1	9.08	126.47	118.30
1	B	72	ASP	CB-CG-OD1	9.04	126.43	118.30
1	A	192	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	A	347	ASP	CB-CG-OD2	-8.79	110.39	118.30
1	B	192	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	B	115	LEU	CB-CG-CD2	8.35	125.20	111.00
1	A	11	ARG	NE-CZ-NH2	-8.29	116.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	B	200	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	19	ARG	NE-CZ-NH1	-8.08	116.26	120.30
1	A	272	ARG	NE-CZ-NH2	8.07	124.33	120.30
1	B	352	PHE	CB-CG-CD2	-8.06	115.16	120.80
1	B	4	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	A	328	ARG	CG-CD-NE	-7.97	95.05	111.80
1	A	200	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	A	4	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	279	ASP	CB-CG-OD2	7.75	125.27	118.30
1	B	192	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	A	214	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	87	GLU	OE1-CD-OE2	-7.53	114.26	123.30
1	A	263	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	A	262	LEU	CB-CG-CD2	7.33	123.45	111.00
1	B	469	VAL	CG1-CB-CG2	-7.12	99.51	110.90
1	A	429	ASP	CB-CG-OD1	7.08	124.67	118.30
1	B	429	ASP	CB-CG-OD1	7.01	124.61	118.30
1	B	157	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	A	70	ARG	NE-CZ-NH1	-6.93	116.83	120.30
1	B	312	ASP	CB-CG-OD1	6.89	124.50	118.30
1	B	199	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	240	GLU	OE1-CD-OE2	-6.80	115.14	123.30
1	A	182	ASP	CB-CG-OD1	-6.76	112.22	118.30
1	B	214	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	A	5	TYR	CB-CG-CD1	6.67	125.00	121.00
1	B	272	ARG	NE-CZ-NH2	6.51	123.56	120.30
1	B	414	GLN	N-CA-CB	-6.45	98.99	110.60
1	B	263	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	B	212	GLY	C-N-CA	-6.34	105.85	121.70
1	A	73	GLU	OE1-CD-OE2	-6.33	115.70	123.30
1	B	87	GLU	OE1-CD-OE2	-6.25	115.80	123.30
1	A	328	ARG	NE-CZ-NH1	-6.23	117.18	120.30
1	B	73	GLU	OE1-CD-OE2	-6.09	115.99	123.30
1	A	199	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	122	LEU	CB-CG-CD2	6.02	121.24	111.00
1	B	210	GLY	N-CA-C	6.01	128.14	113.10
1	B	312	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	B	70	ARG	NE-CZ-NH2	5.99	123.29	120.30
1	B	324	ASP	CB-CG-OD1	5.98	123.68	118.30
1	B	124	ARG	NH1-CZ-NH2	-5.95	112.86	119.40
1	A	375	ASP	CB-CG-OD1	-5.88	113.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	453	PHE	CB-CG-CD1	-5.84	116.71	120.80
1	B	279	ASP	OD1-CG-OD2	-5.84	112.20	123.30
1	A	59	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	A	246	LEU	CB-CG-CD2	-5.83	101.09	111.00
1	A	19	ARG	CG-CD-NE	-5.82	99.58	111.80
1	B	347	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	284	GLU	CB-CG-CD	-5.75	98.68	114.20
1	B	182	ASP	CB-CG-OD1	-5.73	113.14	118.30
1	A	166	GLU	N-CA-CB	5.71	120.88	110.60
1	A	324	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	5	TYR	CB-CG-CD2	-5.66	117.61	121.00
1	A	52	PHE	CB-CG-CD2	5.64	124.75	120.80
1	B	289	LEU	CB-CG-CD2	-5.59	101.49	111.00
1	A	5	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	B	373	TYR	CZ-CE2-CD2	-5.59	114.77	119.80
1	B	283	ARG	NH1-CZ-NH2	5.53	125.48	119.40
1	A	346	LEU	CB-CG-CD1	-5.52	101.62	111.00
1	A	429	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	B	328	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	B	94	GLY	O-C-N	5.42	131.37	122.70
1	A	200	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	166	GLU	CB-CG-CD	-5.39	99.65	114.20
1	A	72	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	339	GLU	OE1-CD-OE2	-5.29	116.96	123.30
1	B	308	VAL	CG1-CB-CG2	-5.24	102.51	110.90
1	B	237	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	352	PHE	CB-CG-CD2	-5.21	117.16	120.80
1	A	156	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	A	367	TYR	CG-CD2-CE2	-5.11	117.22	121.30
1	A	345	ASP	CB-CG-OD1	5.08	122.88	118.30
1	B	381	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	367	TYR	CD1-CE1-CZ	-5.07	115.24	119.80
1	B	59	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	B	236	ARG	CB-CG-CD	-5.05	98.47	111.60
1	B	367	TYR	N-CA-CB	-5.04	101.53	110.60
1	B	391	VAL	CA-CB-CG1	5.04	118.46	110.90
1	B	328	ARG	CB-CG-CD	-5.03	98.51	111.60
1	B	161	LEU	CB-CG-CD1	5.02	119.53	111.00
1	A	367	TYR	CD1-CE1-CZ	-5.01	115.29	119.80

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	3465	0	3425	80	1
1	B	3459	0	3421	78	1
2	A	48	0	26	1	0
2	B	48	0	26	1	0
3	A	9	0	4	0	0
4	A	9	0	4	3	0
4	B	18	0	8	5	0
5	A	6	0	8	6	0
5	B	6	0	8	2	0
6	A	248	0	0	8	0
6	B	256	0	0	8	0
All	All	7572	0	6930	149	1

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 11.

All (149) 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:212:GLY:CA	1:B:433:GLU:O	1.92	1.18
1:A:11:ARG:HG3	1:A:11:ARG:HH21	1.14	1.12
1:A:11:ARG:NH1	1:A:194:SER:O	1.86	1.07
1:B:212:GLY:HA3	1:B:433:GLU:O	1.50	1.07
1:A:217:VAL:H	5:A:479:GOL:H11	1.21	1.00
1:A:341:THR:HA	1:A:344:LEU:HD13	1.42	1.00
1:B:469:VAL:HB	6:B:654:HOH:O	0.82	0.99
1:B:212:GLY:HA2	1:B:433:GLU:O	1.62	0.99
1:A:209:PRO:O	6:A:708:HOH:O	1.81	0.99
1:B:237:ARG:HG2	5:B:479:GOL:O2	1.65	0.95
1:A:212:GLY:HA3	1:A:433:GLU:O	1.64	0.94
1:A:11:ARG:CG	1:A:11:ARG:HH21	1.82	0.93
1:B:262:LEU:O	1:B:266:LEU:HD13	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:HIS:HD2	1:A:92:ASP:H	1.14	0.91
1:A:-1:HIS:NE2	1:A:423:HIS:CD2	2.41	0.89
1:A:-1:HIS:NE2	1:A:423:HIS:CG	2.44	0.85
1:A:217:VAL:H	5:A:479:GOL:C1	1.89	0.84
1:A:362:GLY:H	4:A:478:MLT:H32	1.43	0.83
1:A:11:ARG:NH2	1:A:11:ARG:HG3	1.81	0.81
1:A:402:ALA:HA	1:A:407:VAL:CG1	2.11	0.81
1:B:23:ARG:NH1	1:B:73:GLU:OE1	2.13	0.81
1:B:402:ALA:HA	1:B:407:VAL:CG1	2.10	0.81
1:A:217:VAL:N	5:A:479:GOL:H11	1.96	0.79
1:B:262:LEU:HD23	1:B:266:LEU:HD13	1.65	0.79
1:A:209:PRO:CD	1:B:13:ALA:HB2	2.13	0.78
1:A:209:PRO:HD2	1:B:13:ALA:CB	2.15	0.77
1:A:236:ARG:HG2	1:A:265:GLU:OE2	1.84	0.77
1:A:212:GLY:CA	1:A:433:GLU:O	2.33	0.75
1:A:209:PRO:HG2	1:B:13:ALA:HB2	1.69	0.75
1:A:362:GLY:H	4:A:478:MLT:C3	2.00	0.74
1:B:59:ARG:HB2	1:B:105:LEU:HD12	1.69	0.73
1:A:209:PRO:HD2	1:B:13:ALA:HB2	1.71	0.73
1:B:262:LEU:HD23	1:B:266:LEU:CD1	2.18	0.73
1:B:73:GLU:HG2	6:B:708:HOH:O	1.86	0.72
1:A:-1:HIS:CE1	1:A:423:HIS:CE1	2.78	0.72
1:A:245:HIS:HE1	1:A:274:THR:OG1	1.73	0.72
1:A:203:HIS:HE1	1:A:467:GLU:OE2	1.71	0.71
1:A:6:HIS:NE2	1:A:8:GLU:OE2	2.25	0.69
1:A:209:PRO:CG	1:B:13:ALA:HB2	2.22	0.69
1:A:90:HIS:CD2	1:A:92:ASP:H	2.05	0.69
1:B:73:GLU:OE1	6:B:708:HOH:O	2.09	0.68
1:B:466:PRO:O	1:B:469:VAL:HG23	1.93	0.67
1:B:413:ARG:HG3	1:B:413:ARG:HH11	1.59	0.67
1:B:19:ARG:CB	1:B:19:ARG:HH11	2.08	0.67
1:A:203:HIS:HD2	6:A:549:HOH:O	1.78	0.67
1:A:236:ARG:NE	1:A:265:GLU:OE2	2.28	0.67
1:B:466:PRO:HA	1:B:469:VAL:CG2	2.27	0.65
1:A:391:VAL:HG21	1:A:428:LEU:HD13	1.80	0.64
1:A:209:PRO:HD2	1:B:13:ALA:CA	2.29	0.63
1:B:41:VAL:CG2	1:B:164:LEU:HD11	2.29	0.63
1:B:19:ARG:HH11	1:B:19:ARG:HB2	1.63	0.62
1:B:32:HIS:HE1	6:B:699:HOH:O	1.82	0.62
1:B:41:VAL:HG21	1:B:164:LEU:HD11	1.80	0.62
1:B:237:ARG:HG2	5:B:479:GOL:C2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ARG:NH1	1:B:19:ARG:CB	2.63	0.62
1:B:245:HIS:HE1	1:B:274:THR:OG1	1.81	0.61
1:B:19:ARG:HB3	1:B:19:ARG:NH1	2.15	0.61
1:A:209:PRO:HD2	1:B:13:ALA:HA	1.81	0.61
1:A:55:LYS:HD3	6:A:512:HOH:O	2.00	0.61
1:B:19:ARG:NH2	1:B:45:LEU:O	2.32	0.61
1:A:216:PRO:HA	5:A:479:GOL:H11	1.82	0.61
1:A:236:ARG:CG	1:A:265:GLU:OE2	2.49	0.60
1:B:402:ALA:HA	1:B:407:VAL:HG11	1.82	0.60
1:A:166:GLU:OE2	1:A:166:GLU:CA	2.48	0.60
1:A:77:HIS:HE1	1:A:180:LEU:O	1.84	0.60
1:A:124:ARG:HD2	1:A:166:GLU:HA	1.84	0.59
1:A:212:GLY:N	1:A:433:GLU:O	2.36	0.58
1:A:402:ALA:HA	1:A:407:VAL:HG11	1.83	0.58
1:A:405:PRO:O	1:A:409:ASP:OD2	2.20	0.58
1:B:361:SER:HA	4:B:478:MLT:H2	1.85	0.58
1:A:-1:HIS:NE2	1:A:423:HIS:CE1	2.71	0.58
1:A:-1:HIS:CE1	1:A:423:HIS:ND1	2.73	0.57
1:B:335:ARG:NH2	6:B:553:HOH:O	1.98	0.57
1:A:209:PRO:HG2	1:B:13:ALA:CB	2.34	0.56
1:A:124:ARG:H	1:A:140:GLN:NE2	2.03	0.56
1:B:262:LEU:C	1:B:262:LEU:HD23	2.26	0.56
1:B:73:GLU:CG	6:B:708:HOH:O	2.49	0.56
1:A:-1:HIS:NE2	1:A:423:HIS:NE2	2.54	0.55
1:B:37:TRP:CD1	1:B:124:ARG:HG2	2.41	0.54
1:B:59:ARG:HB2	1:B:105:LEU:CD1	2.38	0.54
1:B:135:LEU:O	1:B:380:HIS:HD2	1.91	0.53
1:B:77:HIS:HE1	1:B:180:LEU:O	1.90	0.53
1:A:220:SER:OG	1:A:245:HIS:HD2	1.91	0.53
1:A:67:ALA:O	1:A:70:ARG:HG3	2.08	0.53
1:B:262:LEU:CD2	1:B:266:LEU:CD1	2.87	0.53
1:A:410:ARG:HG3	1:A:411:LEU:HD23	1.92	0.52
1:A:401:MET:O	1:A:407:VAL:HG11	2.09	0.52
1:A:341:THR:HA	1:A:344:LEU:CD1	2.29	0.52
1:B:438:ALA:HB2	6:B:525:HOH:O	2.09	0.51
1:B:171:ARG:HG2	1:B:175:ARG:NH1	2.26	0.51
1:B:407:VAL:O	1:B:411:LEU:HG	2.10	0.51
1:B:466:PRO:O	1:B:469:VAL:CG2	2.59	0.51
1:A:402:ALA:O	1:A:408:HIS:HB2	2.10	0.51
1:B:41:VAL:CG2	1:B:164:LEU:CD1	2.89	0.51
1:B:23:ARG:HH11	1:B:73:GLU:CD	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:THR:OG1	1:A:304:HIS:HD2	1.94	0.50
1:B:402:ALA:HA	1:B:407:VAL:HG12	1.91	0.50
1:B:152:LEU:HD13	4:B:478:MLT:H31	1.94	0.50
1:A:-2:SER:N	6:A:692:HOH:O	2.27	0.50
1:B:105:LEU:HD13	1:B:108:GLN:OE1	2.12	0.50
1:B:262:LEU:HD23	1:B:262:LEU:O	2.11	0.50
1:B:41:VAL:HG21	1:B:164:LEU:CD1	2.42	0.49
1:B:413:ARG:CG	1:B:413:ARG:HH11	2.23	0.49
1:A:341:THR:CA	1:A:344:LEU:HD13	2.30	0.49
1:A:393:TRP:HB2	2:A:476:NDP:C5N	2.43	0.49
1:B:469:VAL:CB	6:B:654:HOH:O	1.72	0.49
1:A:124:ARG:H	1:A:140:GLN:HE22	1.60	0.48
1:B:409:ASP:O	1:B:413:ARG:HB2	2.12	0.48
1:B:393:TRP:HB2	2:B:476:NDP:C5N	2.44	0.48
1:A:283:ARG:NH1	6:A:679:HOH:O	2.45	0.48
1:A:224:THR:OG1	1:A:304:HIS:CD2	2.67	0.47
1:A:57:THR:OG1	1:A:90:HIS:HE1	1.97	0.47
1:B:362:GLY:H	4:B:478:MLT:C3	2.28	0.47
1:B:262:LEU:C	1:B:262:LEU:CD2	2.83	0.47
1:B:410:ARG:HG3	1:B:411:LEU:HD23	1.98	0.46
1:B:6:HIS:CD2	1:B:8:GLU:HG3	2.50	0.46
1:A:91:THR:HG22	6:A:527:HOH:O	2.15	0.46
1:B:262:LEU:CD2	1:B:266:LEU:HD11	2.46	0.46
1:B:70:ARG:HB2	1:B:115:LEU:HD11	1.98	0.46
1:A:37:TRP:CE2	1:A:124:ARG:HB2	2.51	0.45
1:A:362:GLY:N	4:A:478:MLT:H32	2.23	0.45
1:A:41:VAL:HG21	1:A:164:LEU:HD11	1.99	0.45
1:B:466:PRO:HA	1:B:469:VAL:HG22	1.97	0.45
1:A:355:GLY:HA3	1:A:359:TRP:CZ2	2.52	0.44
1:B:402:ALA:O	1:B:408:HIS:HB2	2.17	0.44
1:A:23:ARG:HH11	1:A:73:GLU:CD	2.20	0.44
1:B:266:LEU:N	1:B:266:LEU:HD12	2.32	0.44
1:B:69:LEU:O	1:B:73:GLU:HB2	2.16	0.44
1:A:135:LEU:O	1:A:380:HIS:HD2	2.00	0.44
1:A:438:ALA:HB2	6:A:674:HOH:O	2.17	0.44
1:B:212:GLY:HA3	1:B:433:GLU:C	2.30	0.44
1:A:37:TRP:CG	1:A:124:ARG:HG3	2.52	0.44
1:A:89:LEU:HD11	1:A:335:ARG:HH22	1.81	0.43
1:A:391:VAL:HG21	1:A:428:LEU:CD1	2.46	0.43
1:A:209:PRO:CG	1:B:13:ALA:CB	2.94	0.43
1:A:283:ARG:NE	6:A:679:HOH:O	2.13	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ASP:O	1:A:413:ARG:HB2	2.18	0.43
1:A:171:ARG:HG2	1:A:175:ARG:NH1	2.34	0.43
1:B:405:PRO:O	1:B:409:ASP:OD2	2.36	0.42
1:B:362:GLY:H	4:B:478:MLT:H2	1.84	0.42
1:A:236:ARG:CD	1:A:265:GLU:OE2	2.67	0.42
1:A:215:PRO:O	5:A:479:GOL:H31	2.20	0.42
1:B:413:ARG:NH1	1:B:413:ARG:HG3	2.28	0.42
1:A:-1:HIS:NE2	1:A:423:HIS:ND1	2.65	0.42
1:B:6:HIS:HD2	1:B:8:GLU:HG3	1.86	0.41
1:B:362:GLY:H	4:B:478:MLT:C2	2.34	0.41
1:B:262:LEU:CD2	1:B:266:LEU:HD13	2.44	0.40
1:A:216:PRO:CA	5:A:479:GOL:H11	2.50	0.40
1:B:364:GLN:N	1:B:365:PRO:CD	2.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ARG:NH1	1:B:311:ASP:OD1[1_664]	1.92	0.28

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%)	465 (98%)	9 (2%)	0	100	100
1	B	473/496 (95%)	464 (98%)	8 (2%)	1 (0%)	47	21
All	All	947/992 (96%)	929 (98%)	17 (2%)	1 (0%)	51	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	394	GLY

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%)	317 (95%)	17 (5%)	24	3
1	B	333/351 (95%)	319 (96%)	14 (4%)	30	5
All	All	667/702 (95%)	636 (95%)	31 (5%)	27	4

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

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	6	HIS
1	A	11	ARG
1	A	19	ARG
1	A	23	ARG
1	A	115	LEU
1	A	124	ARG
1	A	131	ARG
1	A	143	LEU
1	A	166	GLU
1	A	213	LYS
1	A	262	LEU
1	A	311	ASP
1	A	407	VAL
1	A	413	ARG
1	A	421	PRO
1	A	457	ARG
1	B	-2	SER
1	B	-1	HIS
1	B	75	GLU
1	B	82	LEU
1	B	115	LEU
1	B	131	ARG

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Mol	Chain	Res	Type
1	B	143	LEU
1	B	208	VAL
1	B	213	LYS
1	B	284	GLU
1	B	295	GLU
1	B	311	ASP
1	B	409	ASP
1	B	413	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	77	HIS
1	A	90	HIS
1	A	102	GLN
1	A	140	GLN
1	A	203	HIS
1	A	241	GLN
1	A	245	HIS
1	A	304	HIS
1	A	336	HIS
1	A	380	HIS
1	B	32	HIS
1	B	77	HIS
1	B	102	GLN
1	B	241	GLN
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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
5	GOL	A	479	-	5,5,5	1.24	0	5,5,5	1.33	1 (20%)
4	MLT	B	477	-	2,8,8	0.24	0	3,10,10	2.93	2 (66%)
3	LMR	A	477	-	2,8,8	2.26	2 (100%)	3,10,10	4.15	2 (66%)
2	NDP	A	476	-	45,52,52	1.75	12 (26%)	53,80,80	1.43	7 (13%)
5	GOL	B	479	-	5,5,5	0.52	0	5,5,5	0.83	0
2	NDP	B	476	-	45,52,52	1.52	10 (22%)	53,80,80	1.67	9 (16%)
4	MLT	B	478	-	2,8,8	2.28	1 (50%)	3,10,10	4.60	1 (33%)
4	MLT	A	478	-	2,8,8	0.24	0	3,10,10	2.11	2 (66%)

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
5	GOL	A	479	-	-	4/4/4/4	-
4	MLT	B	477	-	-	0/2/8/8	-
3	LMR	A	477	-	-	2/2/8/8	-
2	NDP	A	476	-	-	6/30/77/77	0/5/5/5
5	GOL	B	479	-	-	0/4/4/4	-
2	NDP	B	476	-	-	8/30/77/77	0/5/5/5
4	MLT	B	478	-	-	0/2/8/8	-
4	MLT	A	478	-	-	0/2/8/8	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	476	NDP	C6N-C5N	5.77	1.43	1.33
2	B	476	NDP	C4N-C5N	-4.19	1.38	1.48
2	A	476	NDP	C4N-C5N	-4.03	1.38	1.48
2	A	476	NDP	C3B-C4B	-3.77	1.43	1.53
2	B	476	NDP	C4N-C3N	-3.46	1.43	1.49
2	B	476	NDP	C6N-C5N	3.17	1.39	1.33
4	B	478	MLT	C3-C2	3.11	1.57	1.53
2	A	476	NDP	C2D-C3D	-2.93	1.45	1.53
2	A	476	NDP	P2B-O2B	2.92	1.64	1.59
2	A	476	NDP	C4N-C3N	-2.78	1.44	1.49
2	B	476	NDP	O4D-C1D	2.75	1.48	1.42
2	A	476	NDP	P2B-O2X	-2.61	1.44	1.54
2	B	476	NDP	C3B-C4B	-2.41	1.46	1.53
3	A	477	LMR	O2-C2	-2.38	1.37	1.42
2	B	476	NDP	O4B-C4B	-2.33	1.39	1.45
2	A	476	NDP	C8A-N7A	2.28	1.38	1.34
2	B	476	NDP	C3D-C4D	2.22	1.58	1.53
2	A	476	NDP	O3B-C3B	2.21	1.48	1.43
2	A	476	NDP	C2N-C3N	2.19	1.41	1.34
3	A	477	LMR	C3-C2	-2.12	1.50	1.53
2	B	476	NDP	P2B-O2X	-2.08	1.46	1.54
2	A	476	NDP	O4D-C1D	2.08	1.46	1.42
2	A	476	NDP	C2A-N3A	2.06	1.35	1.32
2	B	476	NDP	C2N-C3N	2.05	1.40	1.34
2	B	476	NDP	PN-O2N	-2.04	1.45	1.55

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	478	MLT	C3-C2-C1	7.94	121.20	111.10
2	B	476	NDP	N3A-C2A-N1A	-5.49	120.10	128.68
3	A	477	LMR	C3-C2-C1	5.07	117.55	111.10
3	A	477	LMR	O2-C2-C1	-4.77	97.30	111.66
4	B	477	MLT	C3-C2-C1	-4.17	105.79	111.10
2	A	476	NDP	C4A-C5A-N7A	-3.95	105.28	109.40
2	B	476	NDP	C2A-N1A-C6A	3.75	125.17	118.75
2	B	476	NDP	O2B-P2B-O1X	-3.16	97.20	109.39
2	B	476	NDP	C3N-C2N-N1N	-3.15	118.60	123.10
2	A	476	NDP	O2B-P2B-O1X	-3.11	97.38	109.39
2	B	476	NDP	O4B-C4B-C3B	3.03	111.12	105.11
2	A	476	NDP	N3A-C2A-N1A	-3.01	123.97	128.68
2	B	476	NDP	N6A-C6A-N1A	3.01	124.82	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	476	NDP	O4B-C4B-C3B	2.88	110.81	105.11
4	A	478	MLT	O3-C2-C1	-2.87	103.02	111.66
4	B	477	MLT	O3-C2-C1	-2.73	103.46	111.66
2	B	476	NDP	C5A-C6A-N1A	-2.65	114.34	120.35
2	A	476	NDP	O4D-C1D-C2D	-2.57	101.05	106.64
2	A	476	NDP	C5A-C6A-N6A	2.29	123.83	120.35
2	B	476	NDP	O3B-C3B-C4B	-2.26	104.50	111.05
2	A	476	NDP	C3N-C2N-N1N	-2.18	119.98	123.10
5	A	479	GOL	C3-C2-C1	2.17	120.14	111.70
4	A	478	MLT	O3-C2-C3	2.13	113.17	108.50
2	B	476	NDP	C1B-N9A-C4A	-2.10	122.96	126.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

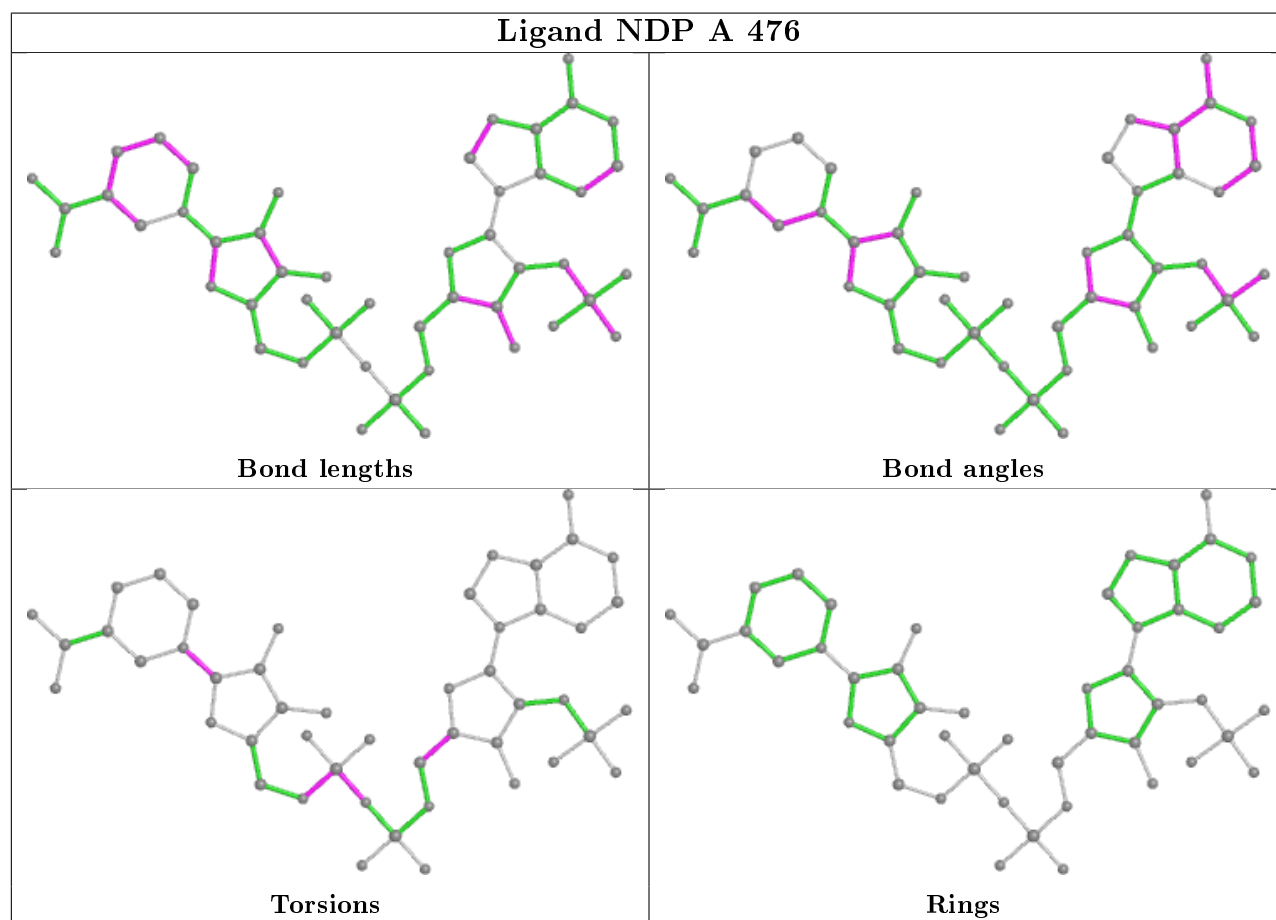
Mol	Chain	Res	Type	Atoms
5	A	479	GOL	O1-C1-C2-C3
5	A	479	GOL	C1-C2-C3-O3
5	A	479	GOL	O2-C2-C3-O3
3	A	477	LMR	O2-C2-C3-C4
2	A	476	NDP	C5D-O5D-PN-O2N
2	B	476	NDP	C5D-O5D-PN-O2N
2	A	476	NDP	O4D-C1D-N1N-C6N
2	B	476	NDP	O4D-C1D-N1N-C6N
5	A	479	GOL	O1-C1-C2-O2
2	A	476	NDP	C5D-O5D-PN-O3
2	B	476	NDP	C5D-O5D-PN-O3
2	A	476	NDP	C5D-O5D-PN-O1N
2	B	476	NDP	C5D-O5D-PN-O1N
3	A	477	LMR	C1-C2-C3-C4
2	B	476	NDP	PA-O3-PN-O2N
2	A	476	NDP	PA-O3-PN-O2N
2	B	476	NDP	C3B-C2B-O2B-P2B
2	B	476	NDP	C2N-C3N-C7N-N7N
2	A	476	NDP	O4B-C4B-C5B-O5B
2	B	476	NDP	O4B-C4B-C5B-O5B

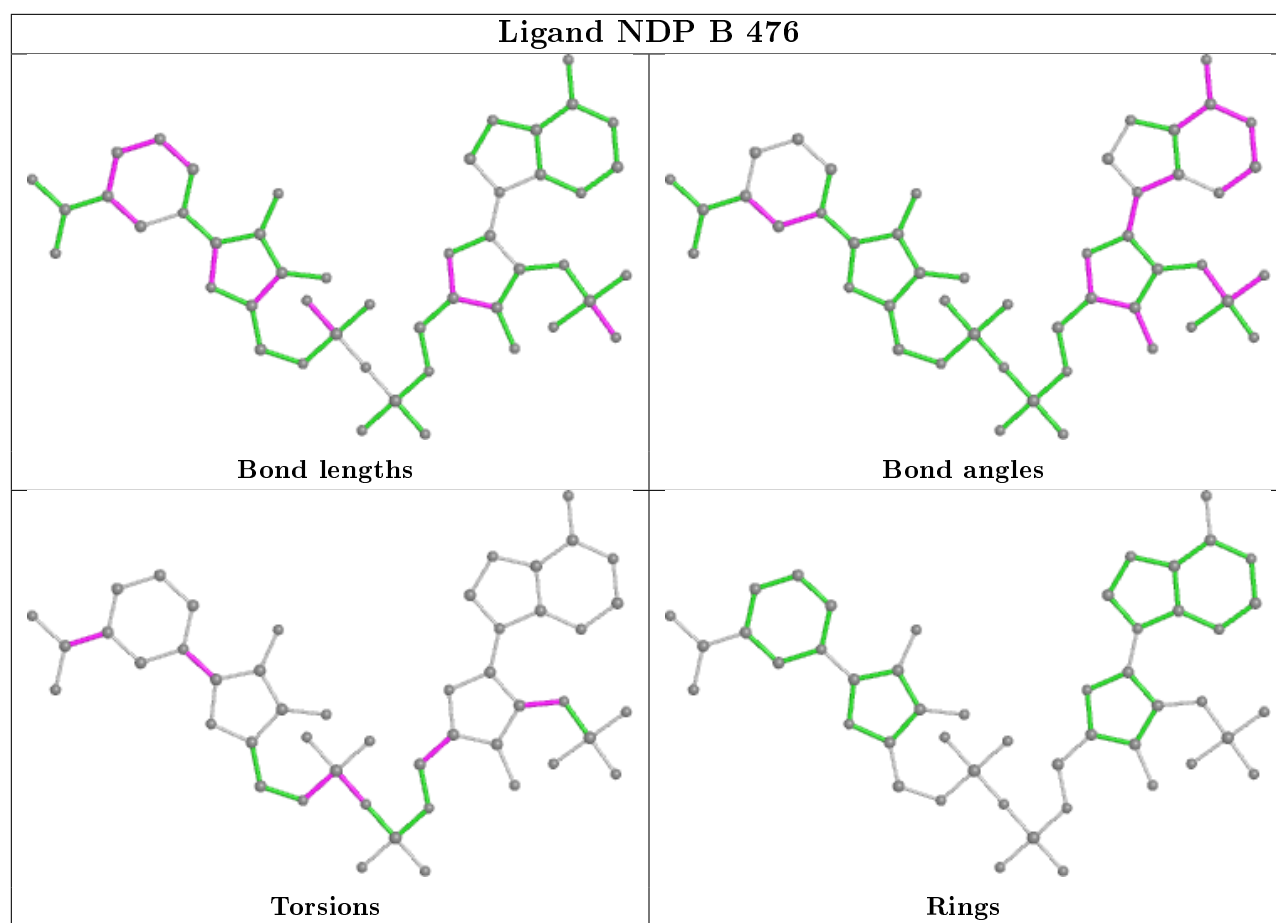
There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	479	GOL	6	0
2	A	476	NDP	1	0
5	B	479	GOL	2	0
2	B	476	NDP	1	0
4	B	478	MLT	5	0
4	A	478	MLT	3	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%)	0.32	34 (7%) 16 14	8, 15, 35, 58	0
1	B	475/496 (95%)	0.34	28 (5%) 22 20	8, 15, 35, 59	0
All	All	951/992 (95%)	0.33	62 (6%) 18 17	8, 15, 35, 59	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	210	GLY	9.6
1	B	212	GLY	9.1
1	B	213	LYS	8.2
1	B	211	SER	6.4
1	A	210	GLY	6.3
1	A	406	GLU	5.9
1	A	212	GLY	5.8
1	B	209	PRO	5.8
1	A	209	PRO	5.8
1	A	413	ARG	5.6
1	A	407	VAL	5.4
1	A	295	GLU	5.0
1	A	213	LYS	5.0
1	A	211	SER	4.8
1	B	406	GLU	4.7
1	B	208	VAL	4.6
1	A	208	VAL	4.4
1	A	411	LEU	4.3
1	B	412	VAL	4.2
1	A	131	ARG	4.2
1	B	413	ARG	4.2
1	B	-1	HIS	3.9
1	B	411	LEU	3.9
1	A	409	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	70	ARG	3.4
1	B	131	ARG	3.4
1	B	74	GLY	3.2
1	A	-1	HIS	3.2
1	A	412	VAL	3.1
1	B	410	ARG	3.1
1	A	71	GLU	3.1
1	A	70	ARG	3.0
1	A	410	ARG	3.0
1	B	55	LYS	2.9
1	A	171	ARG	2.9
1	B	171	ARG	2.8
1	A	72	ASP	2.8
1	A	11	ARG	2.7
1	A	74	GLY	2.7
1	A	405	PRO	2.6
1	B	405	PRO	2.6
1	B	295	GLU	2.6
1	B	407	VAL	2.5
1	B	75	GLU	2.5
1	A	404	ASP	2.5
1	B	414	GLN	2.5
1	A	296	ASP	2.4
1	B	402	ALA	2.4
1	A	414	GLN	2.3
1	A	166	GLU	2.3
1	B	409	ASP	2.3
1	B	166	GLU	2.2
1	A	408	HIS	2.2
1	A	21	ALA	2.2
1	B	71	GLU	2.2
1	A	55	LYS	2.1
1	A	294	PRO	2.1
1	A	403	THR	2.1
1	B	342	ALA	2.1
1	A	343	ASP	2.0
1	A	342	ALA	2.0
1	B	48	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

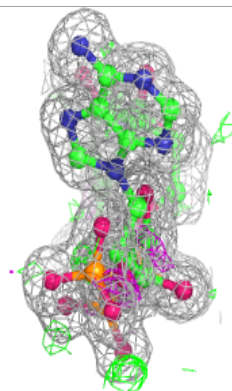
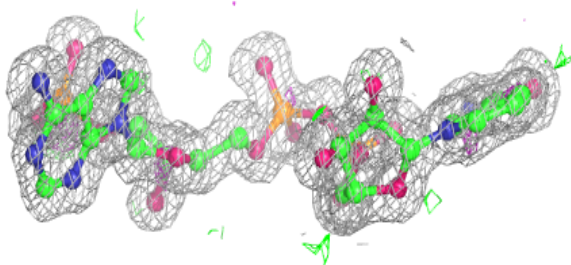
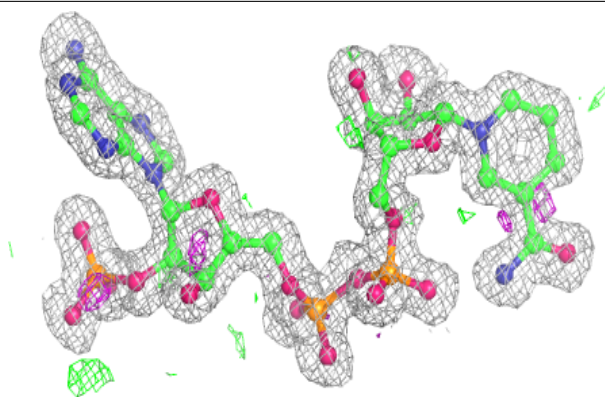
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MLT	B	478	9/9	0.77	0.15	31,42,50,52	0
4	MLT	A	478	9/9	0.77	0.21	27,37,44,45	0
5	GOL	A	479	6/6	0.81	0.17	26,29,35,36	0
3	LMR	A	477	9/9	0.82	0.23	24,42,47,49	0
5	GOL	B	479	6/6	0.83	0.17	24,32,35,37	0
4	MLT	B	477	9/9	0.84	0.19	26,41,47,47	0
2	NDP	A	476	48/48	0.97	0.07	10,13,16,18	0
2	NDP	B	476	48/48	0.98	0.07	9,12,15,17	0

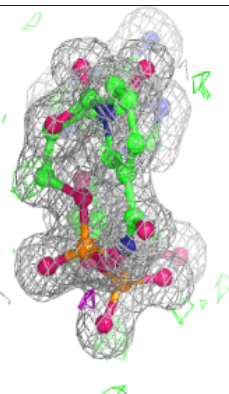
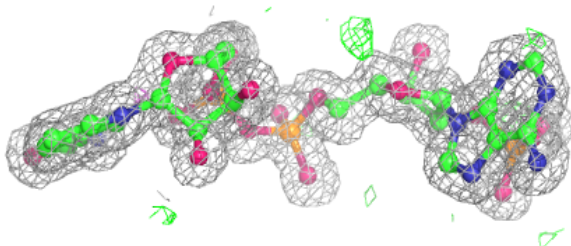
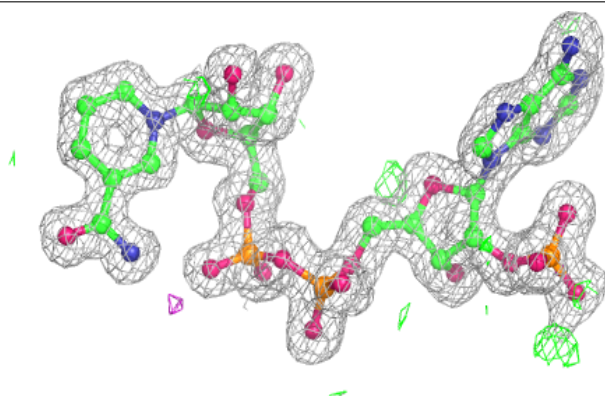
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

There are no such residues in this entry.