



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:37 am GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

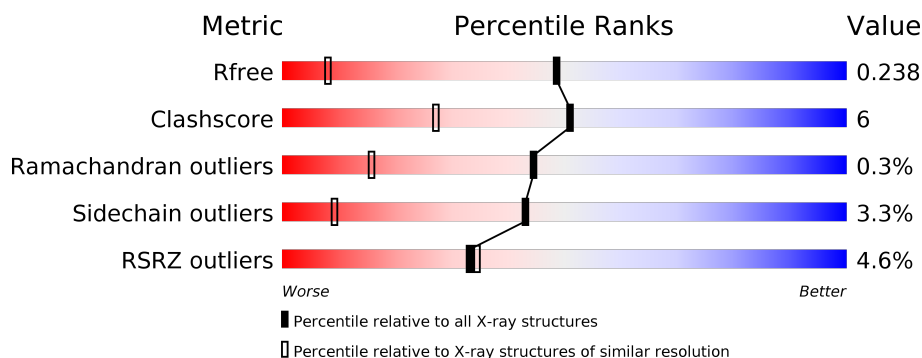
1 Overall quality at a glance

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}	100719	1510 (1.48-1.44)
Clashscore	112137	1573 (1.48-1.44)
Ramachandran outliers	110173	1555 (1.48-1.44)
Sidechain outliers	110143	1555 (1.48-1.44)
RSRZ outliers	101464	1516 (1.48-1.44)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	496	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• •</div> </div> </div>
1	B	496	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>• •</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NDP	A	476	X	-	-	-
2	NDP	B	476	X	-	-	-

2 Entry composition

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:

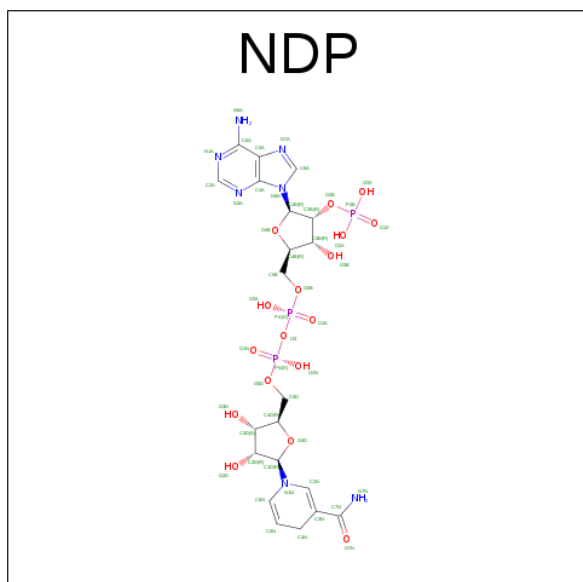
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q93NW7
A	-19	GLY	-	EXPRESSION TAG	UNP Q93NW7
A	-18	SER	-	EXPRESSION TAG	UNP Q93NW7
A	-17	SER	-	EXPRESSION TAG	UNP Q93NW7
A	-16	HIS	-	EXPRESSION TAG	UNP Q93NW7
A	-15	HIS	-	EXPRESSION TAG	UNP Q93NW7
A	-14	HIS	-	EXPRESSION TAG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

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

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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		

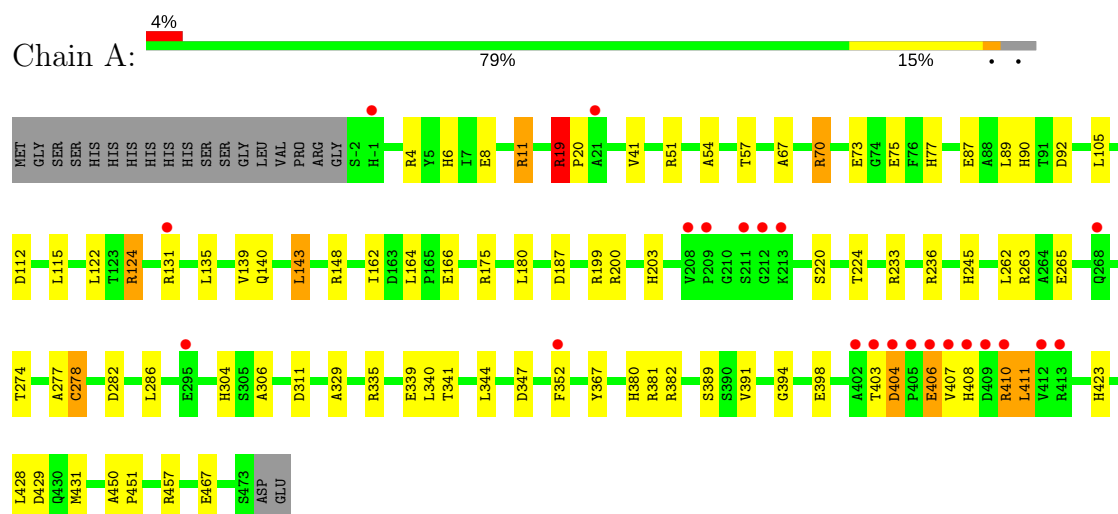
- Molecule 3 is water.

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

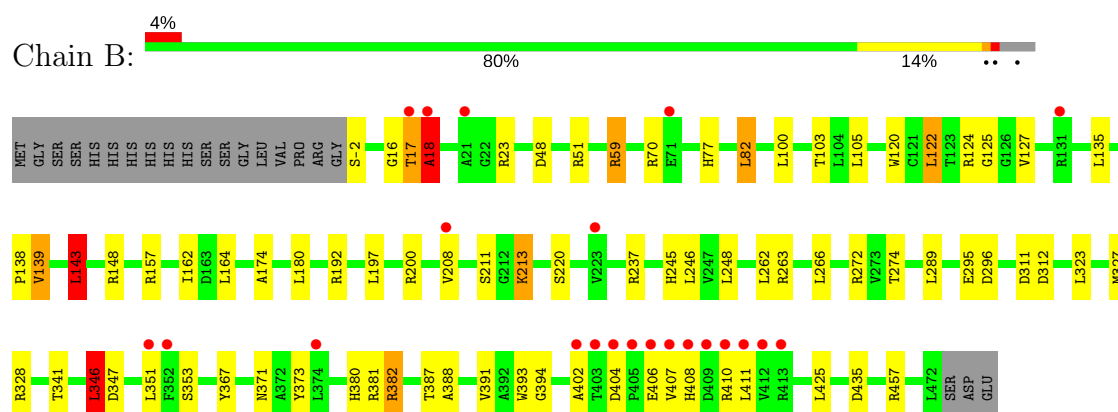
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: AmphB



• Molecule 1: AmphB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.50Å 63.69Å 71.92Å 72.93° 67.21° 89.76°	Depositor
Resolution (Å)	50.00 – 1.46 26.60 – 1.46	Depositor EDS
% Data completeness (in resolution range)	82.9 (50.00-1.46) 72.8 (26.60-1.46)	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 (5.27%)	DCC
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.4	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	0.95	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	1.26	9/3531 (0.3%)	1.24	28/4822 (0.6%)
1	B	1.26	9/3525 (0.3%)	1.35	39/4814 (0.8%)
All	All	1.26	18/7056 (0.3%)	1.29	67/9636 (0.7%)

All (18) bond length outliers are listed below:

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

All (67) bond angle outliers are listed below:

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

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

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLU:C	1:A:403:THR:HG21	2.37	0.44
1:A:122:LEU:HD22	1:A:162:ILE:HB	2.00	0.43
1:B:122:LEU:HD22	1:B:162:ILE:HB	1.99	0.43
1:A:286:LEU:HD23	1:A:340:LEU:HD12	2.00	0.43
1:A:406:GLU:HB3	1:A:407:VAL:H	1.48	0.42
1:B:394:GLY:O	2:B:476:NDP:H42N	2.19	0.42
1:B:341:THR:HB	1:B:346:LEU:CD2	2.50	0.42
1:B:353:SER:HA	1:B:371:ASN:OD1	2.19	0.42
1:A:19:ARG:HE	1:A:19:ARG:HB2	1.39	0.42
1:B:100:LEU:HA	1:B:143:LEU:HD22	2.01	0.42
1:B:262:LEU:HD23	1:B:262:LEU:O	2.20	0.41
1:A:115:LEU:N	1:A:115:LEU:HD12	2.36	0.41
1:B:138:PRO:HB2	1:B:373:TYR:CE1	2.56	0.41
1:B:407:VAL:O	1:B:411:LEU:HD12	2.20	0.41
1:A:450:ALA:HB3	1:A:451:PRO:HD3	2.02	0.41
1:B:323:LEU:O	1:B:327:MET:HG2	2.21	0.41
1:B:135:LEU:O	1:B:380:HIS:CD2	2.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	474/496 (96%)	458 (97%)	15 (3%)	1 (0%)	51	21
1	B	473/496 (95%)	462 (98%)	9 (2%)	2 (0%)	38	12
All	All	947/992 (96%)	920 (97%)	24 (2%)	3 (0%)	44	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLU

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/351 (95%)	322 (96%)	12 (4%)	40	7
1	B	333/351 (95%)	323 (97%)	10 (3%)	46	11
All	All	667/702 (95%)	645 (97%)	22 (3%)	43	9

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

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

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Mol	Chain	Res	Type
1	B	410	ARG

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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	A	476	-	43,52,52	1.40	5 (11%)	49,80,80	2.43	11 (22%)
2	NDP	B	476	-	43,52,52	1.41	5 (11%)	49,80,80	2.79	13 (26%)

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	476	NDP	C4N-C5N	-3.77	1.40	1.49
2	A	476	NDP	C4N-C5N	-3.73	1.41	1.49
2	B	476	NDP	O7N-C7N	-2.68	1.17	1.24
2	A	476	NDP	C6N-N1N	-2.08	1.31	1.37
2	A	476	NDP	O4D-C1D	2.34	1.47	1.42
2	B	476	NDP	C6N-C5N	2.37	1.37	1.33
2	B	476	NDP	P2B-O2B	3.11	1.65	1.59
2	A	476	NDP	C6N-C5N	3.37	1.39	1.33
2	A	476	NDP	P2B-O2B	3.91	1.66	1.59
2	B	476	NDP	C4A-N3A	3.96	1.41	1.35

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	476	NDP	N3A-C2A-N1A	-11.50	118.84	128.86
2	A	476	NDP	N3A-C2A-N1A	-8.81	121.18	128.86
2	B	476	NDP	C4B-O4B-C1B	-7.09	102.22	109.77
2	B	476	NDP	C2B-C3B-C4B	-7.03	85.97	101.95
2	A	476	NDP	C4B-O4B-C1B	-6.80	102.53	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	476	NDP	C2B-C3B-C4B	-6.61	86.93	101.95
2	B	476	NDP	C1B-N9A-C4A	-3.64	120.34	126.64
2	B	476	NDP	O2B-P2B-O1X	-3.28	96.41	109.26
2	B	476	NDP	O4B-C1B-C2B	-2.90	101.52	106.59
2	A	476	NDP	C1B-N9A-C4A	-2.69	121.99	126.64
2	B	476	NDP	C1D-N1N-C6N	-2.60	115.12	120.77
2	A	476	NDP	O2B-P2B-O1X	-2.43	99.75	109.26
2	A	476	NDP	O4B-C1B-C2B	-2.06	102.99	106.59
2	B	476	NDP	O2A-PA-O1A	2.07	122.99	112.28
2	B	476	NDP	O3X-P2B-O2X	2.18	116.40	107.61
2	A	476	NDP	O4B-C4B-C5B	2.46	117.69	109.40
2	A	476	NDP	C2A-N1A-C6A	2.73	123.56	118.77
2	B	476	NDP	O3B-C3B-C4B	2.80	119.26	111.09
2	A	476	NDP	C5B-C4B-C3B	2.87	126.21	115.29
2	A	476	NDP	O3B-C3B-C4B	3.04	119.96	111.09
2	B	476	NDP	C5B-C4B-C3B	3.52	128.71	115.29
2	B	476	NDP	O4B-C4B-C3B	4.45	114.01	105.17
2	B	476	NDP	C2A-N1A-C6A	4.93	127.39	118.77
2	A	476	NDP	O4B-C4B-C3B	5.49	116.09	105.17

All (2) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	476	NDP	1	0
2	B	476	NDP	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.12	22 (4%) 33 34	9, 16, 32, 67	0
1	B	475/496 (95%)	0.12	22 (4%) 33 34	8, 15, 30, 64	0
All	All	951/992 (95%)	0.12	44 (4%) 33 34	8, 16, 32, 67	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	VAL	7.5
1	B	405	PRO	6.6
1	A	402	ALA	6.3
1	A	405	PRO	5.8
1	A	404	ASP	5.1
1	A	403	THR	4.7
1	B	17	THR	4.2
1	A	406	GLU	4.2
1	B	131	ARG	3.9
1	A	408	HIS	3.8
1	B	411	LEU	3.7
1	B	18	ALA	3.7
1	A	131	ARG	3.5
1	A	413	ARG	3.4
1	B	408	HIS	3.4
1	A	213	LYS	3.3
1	A	410	ARG	3.2
1	B	406	GLU	3.1
1	B	407	VAL	3.1
1	A	208	VAL	3.0
1	A	409	ASP	3.0
1	A	412	VAL	3.0
1	B	409	ASP	3.0
1	B	413	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	352	PHE	2.8
1	B	403	THR	2.7
1	B	412	VAL	2.6
1	B	352	PHE	2.6
1	A	212	GLY	2.5
1	A	209	PRO	2.4
1	A	295	GLU	2.3
1	B	351	LEU	2.3
1	B	71	GLU	2.3
1	B	404	ASP	2.3
1	B	21	ALA	2.2
1	A	211	SER	2.2
1	B	402	ALA	2.2
1	B	374	LEU	2.2
1	B	208	VAL	2.2
1	A	268	GLN	2.1
1	B	410	ARG	2.1
1	A	-1	HIS	2.1
1	B	223	VAL	2.1
1	A	21	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	NDP	A	476	48/48	0.96	0.11	0.11	16,21,25,25	0
2	NDP	B	476	48/48	0.98	0.07	-0.75	12,17,20,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.