



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 02:04 AM EDT

PDB ID : 3P9O
Title : Aerobic ternary complex of urate oxidase with azide and chloride
Authors : Gabison, L.; Colloc'H, N.; El Hajji, M.; Castro, B.; Chiadmi, M.; Prange, T.
Deposited on : 2010-10-18
Resolution : 1.45 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

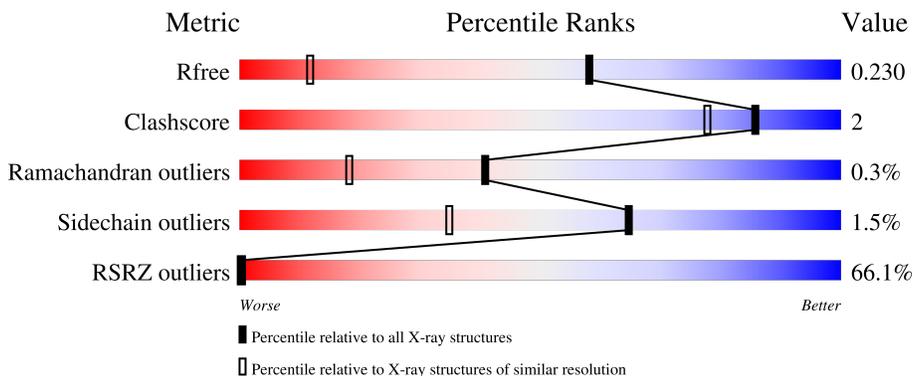
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	302	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2826 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.

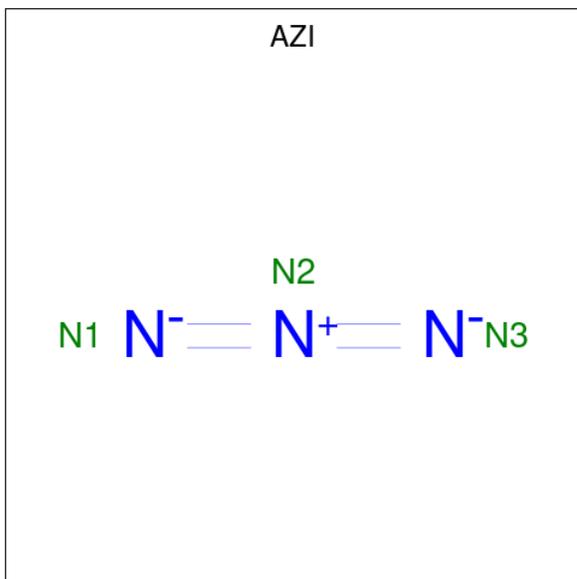
- Molecule 1 is a protein called Uricase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2429	1531	424	463	11	0	18	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	acetylation	UNP Q00511

- Molecule 2 is AZIDE ION (three-letter code: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	N	0	0
			3	3		
2	A	1	Total	N	0	0
			3	3		
2	A	1	Total	N	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total N 3 3	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0

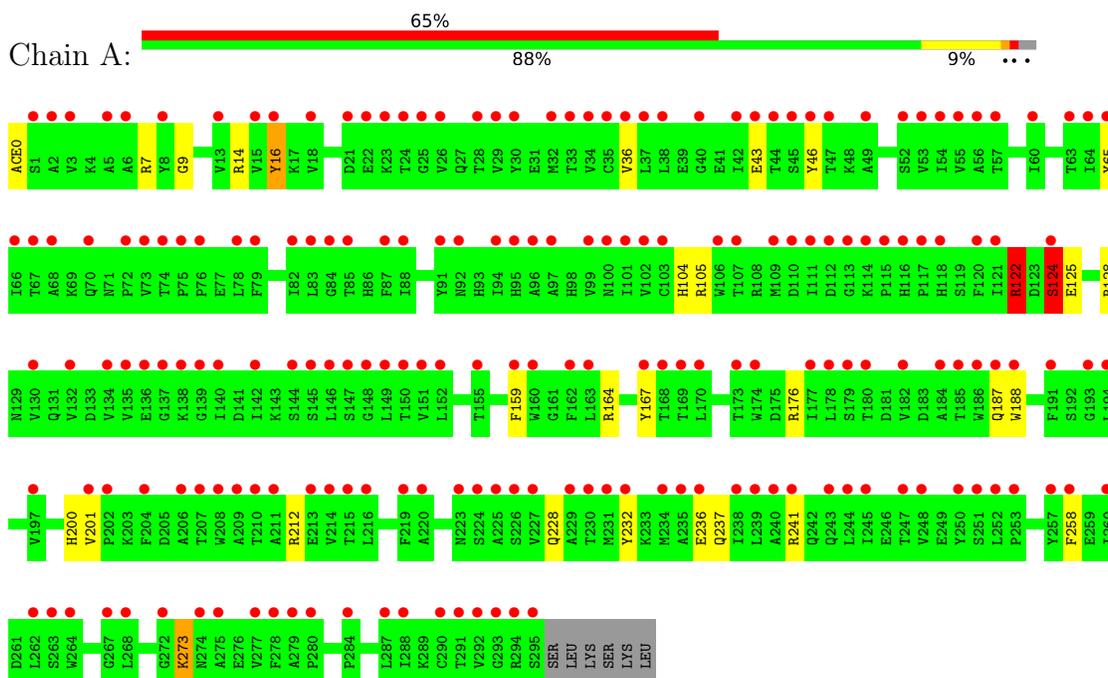
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	383	Total O 383 383	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: Uricase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	79.49Å 94.99Å 104.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.70 – 1.45 39.75 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.70-1.45) 99.4 (39.75-1.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.75 (at 1.45Å)	Xtrriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.201 , 0.255 0.231 , 0.230	Depositor DCC
R_{free} test set	4287 reflections (6.13%)	wwPDB-VP
Wilson B-factor (Å ²)	2.5	Xtrriage
Anisotropy	1.716	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.29$, $\langle L^2 \rangle = 0.13$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2826	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: CL, AZI, NA, ACE

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	0.68	1/2570 (0.0%)	1.49	31/3476 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	0	ACE	C-N	5.74	1.47	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ARG	NE-CZ-NH1	15.44	128.02	120.30
1	A	188	TRP	CD1-NE1-CE2	11.98	119.79	109.00
1	A	104	HIS	CG-ND1-CE1	10.42	122.79	108.20
1	A	14	ARG	NE-CZ-NH1	-8.69	115.95	120.30
1	A	212	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	122[A]	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	122[B]	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	164	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	A	16	TYR	CB-CG-CD1	8.22	125.93	121.00
1	A	128	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	A	176	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	A	7	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	A	7	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	A	228	GLN	O-C-N	-7.24	111.11	122.70
1	A	188	TRP	NE1-CE2-CD2	-7.19	100.11	107.30
1	A	65	TYR	CB-CG-CD1	-6.99	116.81	121.00
1	A	188	TRP	CG-CD1-NE1	-6.96	103.14	110.10
1	A	124	SER	O-C-N	6.94	133.81	122.70
1	A	212	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	104	HIS	ND1-CG-CD2	-6.58	96.79	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	TYR	CG-CD1-CE1	6.21	126.27	121.30
1	A	16	TYR	CG-CD1-CE1	6.13	126.21	121.30
1	A	188	TRP	NE1-CE2-CZ2	6.04	137.05	130.40
1	A	159	PHE	CB-CG-CD1	-5.94	116.64	120.80
1	A	128	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	14	ARG	NH1-CZ-NH2	5.67	125.64	119.40
1	A	46	TYR	CZ-CE2-CD2	5.60	124.84	119.80
1	A	200	HIS	CG-ND1-CE1	5.54	115.96	108.20
1	A	258	PHE	CG-CD2-CE2	5.37	126.70	120.80
1	A	167	TYR	CB-CG-CD1	5.18	124.11	121.00
1	A	105	ARG	NE-CZ-NH2	5.15	122.87	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2429	0	2421	11	0
2	A	12	0	0	1	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	383	0	0	4	0
All	All	2826	0	2421	11	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 2.

All (11) 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:A:273[A]:LYS:HD2	5:A:1169:HOH:O	1.86	0.76
1:A:124:SER:HB2	5:A:1188:HOH:O	1.90	0.71
1:A:237:GLN:O	1:A:241[A]:ARG:HG3	1.90	0.70
1:A:273[A]:LYS:HE3	5:A:1345:HOH:O	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLN:HG2	2:A:304:AZI:N3	2.17	0.59
1:A:232:TYR:O	1:A:236[B]:GLU:HG3	2.11	0.49
1:A:122[B]:ARG:NH1	5:A:1346:HOH:O	2.49	0.45
1:A:122[A]:ARG:HD2	1:A:125:GLU:OE1	2.17	0.45
1:A:9:GLY:HA3	1:A:36:VAL:O	2.19	0.43
1:A:43:GLU:CD	1:A:43:GLU:H	2.23	0.41

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	312/302 (103%)	306 (98%)	5 (2%)	1 (0%)	41 18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	SER

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	279/267 (104%)	273 (98%)	6 (2%)	52 18

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	TYR
1	A	122[A]	ARG
1	A	122[B]	ARG
1	A	124	SER
1	A	273[A]	LYS
1	A	273[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	100	ASN
1	A	129	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	AZI	A	305	-	0,2,2	-	-	0,1,1	-	-
2	AZI	A	303	-	0,2,2	-	-	0,1,1	-	-
2	AZI	A	302	-	0,2,2	-	-	0,1,1	-	-
2	AZI	A	304	-	0,2,2	-	-	0,1,1	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	304	AZI	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	295/302 (97%)	2.51	195 (66%) 0 0	9, 13, 26, 50	2 (0%)

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	LYS	6.5
1	A	113	GLY	6.4
1	A	137	GLY	6.4
1	A	22[A]	GLU	6.0
1	A	295	SER	5.3
1	A	288	ILE	4.8
1	A	174	TRP	4.4
1	A	188	TRP	4.4
1	A	245	ILE	4.4
1	A	112	ASP	4.2
1	A	64	ILE	4.2
1	A	204	PHE	4.1
1	A	111	ILE	4.1
1	A	121	ILE	4.1
1	A	290[A]	CYS	4.0
1	A	248	VAL	4.0
1	A	24	THR	4.0
1	A	239	LEU	4.0
1	A	103[A]	CYS	3.9
1	A	208	TRP	3.8
1	A	138[A]	LYS	3.8
1	A	186	TRP	3.8
1	A	142	ILE	3.8
1	A	53	VAL	3.8
1	A	152	LEU	3.7
1	A	106	TRP	3.7
1	A	160	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	102	VAL	3.7
1	A	140	ILE	3.7
1	A	16	TYR	3.7
1	A	96	ALA	3.7
1	A	66	ILE	3.7
1	A	32[A]	MET	3.7
1	A	92	ASN	3.7
1	A	132	VAL	3.6
1	A	79	PHE	3.6
1	A	120	PHE	3.6
1	A	60	ILE	3.6
1	A	38	LEU	3.6
1	A	191	PHE	3.5
1	A	229	ALA	3.5
1	A	91	TYR	3.5
1	A	88	ILE	3.5
1	A	209	ALA	3.5
1	A	99	VAL	3.5
1	A	278	PHE	3.5
1	A	177	ILE	3.4
1	A	262	LEU	3.4
1	A	159	PHE	3.4
1	A	287	LEU	3.3
1	A	65	TYR	3.3
1	A	34	VAL	3.3
1	A	134	VAL	3.3
1	A	115	PRO	3.3
1	A	258	PHE	3.3
1	A	35	CYS	3.3
1	A	26	VAL	3.3
1	A	197	VAL	3.3
1	A	78	LEU	3.3
1	A	82	ILE	3.3
1	A	18	VAL	3.3
1	A	135	VAL	3.3
1	A	257	TYR	3.3
1	A	163	LEU	3.3
1	A	268	LEU	3.3
1	A	101	ILE	3.2
1	A	36	VAL	3.2
1	A	21	ASP	3.2
1	A	117	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1	SER	3.2
1	A	130	VAL	3.2
1	A	292	VAL	3.2
1	A	8	TYR	3.2
1	A	180	THR	3.1
1	A	216	LEU	3.1
1	A	244	LEU	3.1
1	A	15	VAL	3.1
1	A	250	TYR	3.1
1	A	87	PHE	3.1
1	A	25	GLY	3.1
1	A	124	SER	3.1
1	A	214	VAL	3.1
1	A	42	ILE	3.1
1	A	54	ILE	3.1
1	A	232	TYR	3.1
1	A	74	THR	3.1
1	A	146	LEU	3.0
1	A	114	LYS	3.0
1	A	13	VAL	3.0
1	A	83	LEU	3.0
1	A	3	VAL	3.0
1	A	184	ALA	3.0
1	A	252	LEU	3.0
1	A	215	THR	2.9
1	A	75	PRO	2.9
1	A	227	VAL	2.9
1	A	46	TYR	2.9
1	A	260	ILE	2.9
1	A	194	LEU	2.9
1	A	277	VAL	2.9
1	A	118	HIS	2.9
1	A	110	ASP	2.9
1	A	264	TRP	2.9
1	A	240	ALA	2.8
1	A	73	VAL	2.8
1	A	136	GLU	2.8
1	A	274	ASN	2.8
1	A	2	ALA	2.8
1	A	162	PHE	2.8
1	A	234	MET	2.8
1	A	149	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	275	ALA	2.8
1	A	148	GLY	2.8
1	A	219	PHE	2.8
1	A	30	TYR	2.8
1	A	207	THR	2.7
1	A	291	THR	2.7
1	A	155	THR	2.7
1	A	37	LEU	2.7
1	A	170	LEU	2.7
1	A	238	ILE	2.7
1	A	5	ALA	2.7
1	A	97	ALA	2.7
1	A	279	ALA	2.7
1	A	116	HIS	2.7
1	A	55	VAL	2.7
1	A	72	PRO	2.7
1	A	56	ALA	2.7
1	A	206	ALA	2.7
1	A	173	THR	2.6
1	A	280	PRO	2.6
1	A	28	THR	2.6
1	A	33	THR	2.6
1	A	243	GLN	2.6
1	A	45	SER	2.6
1	A	70[A]	GLN	2.6
1	A	293	GLY	2.6
1	A	235	ALA	2.6
1	A	84	GLY	2.5
1	A	167	TYR	2.5
1	A	178	LEU	2.5
1	A	182	VAL	2.5
1	A	251	SER	2.5
1	A	267	GLY	2.5
1	A	109	MET	2.5
1	A	147	SER	2.4
1	A	44	THR	2.4
1	A	211	ALA	2.4
1	A	185	THR	2.4
1	A	247	THR	2.4
1	A	263	SER	2.4
1	A	95	HIS	2.4
1	A	187	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	68	ALA	2.4
1	A	231[A]	MET	2.4
1	A	57	THR	2.4
1	A	150	THR	2.4
1	A	144	SER	2.4
1	A	47	THR	2.4
1	A	201	VAL	2.3
1	A	85	THR	2.3
1	A	94	ILE	2.3
1	A	236[A]	GLU	2.3
1	A	29	VAL	2.3
1	A	253	PRO	2.3
1	A	76	PRO	2.2
1	A	210	THR	2.2
1	A	241[A]	ARG	2.2
1	A	43	GLU	2.2
1	A	226	SER	2.2
1	A	220	ALA	2.2
1	A	100	ASN	2.2
1	A	272	GLY	2.2
1	A	49	ALA	2.2
1	A	63	THR	2.2
1	A	179	SER	2.2
1	A	224	SER	2.2
1	A	40	GLY	2.2
1	A	294	ARG	2.2
1	A	151	VAL	2.2
1	A	223	ASN	2.1
1	A	202	PRO	2.1
1	A	213	GLU	2.1
1	A	6	ALA	2.1
1	A	52	SER	2.1
1	A	145	SER	2.1
1	A	193	GLY	2.1
1	A	168	THR	2.1
1	A	169	THR	2.1
1	A	230	THR	2.1
1	A	284	PRO	2.1
1	A	107	THR	2.1
1	A	139	GLY	2.1
1	A	67	THR	2.0
1	A	225	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, 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
2	AZI	A	305	3/3	0.49	0.39	30,30,35,46	0
2	AZI	A	304	3/3	0.81	0.21	26,26,34,45	0
2	AZI	A	303	3/3	0.91	0.18	14,14,24,25	0
2	AZI	A	302	3/3	0.94	0.17	12,12,15,16	0
4	NA	A	502	1/1	0.97	0.15	14,14,14,14	0
3	CL	A	501	1/1	0.99	0.14	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.