



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:36 am BST

PDB ID : 5W57
Title : Structure of Holo AztC
Authors : Avalos, D.; Yukl, E.T.
Deposited on : 2017-06-14
Resolution : 2.30 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

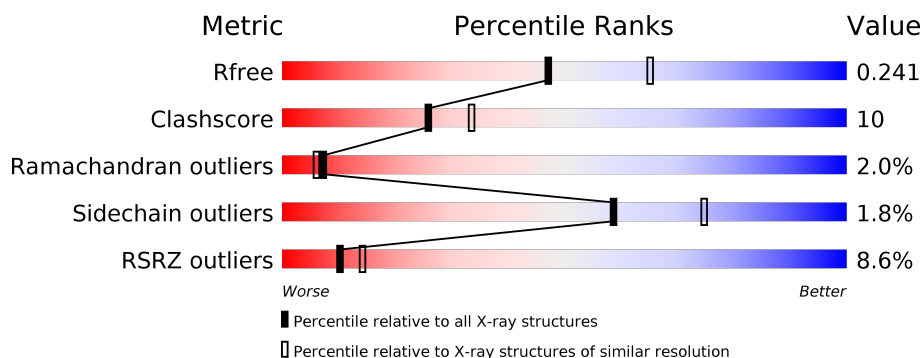
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	286	<div> <div>10%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>..</div> </div> </div>
1	B	286	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>..</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4240 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 Periplasmic solute binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2081	1305	365	406	5			
1	B	284	Total	C	N	O	S	0	2	0
			2106	1320	371	410	5			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

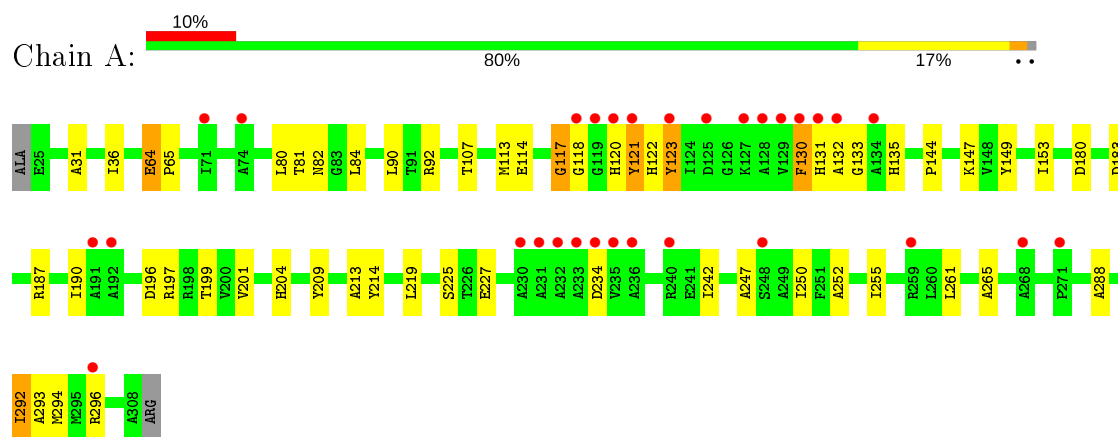
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		
3	B	29	Total	O	0	0
			29	29		

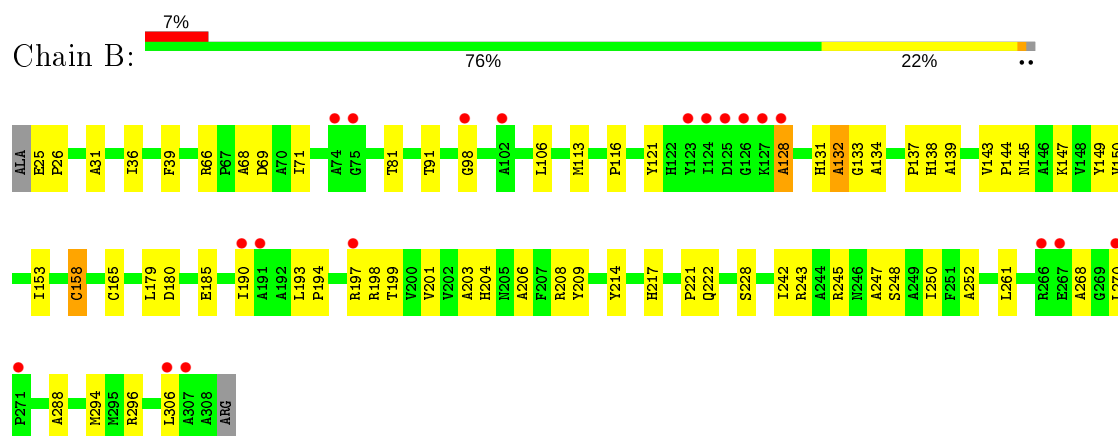
3 Residue-property plots [i](#)

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: Periplasmic solute binding protein



• Molecule 1: Periplasmic solute binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.84Å 72.37Å 105.61Å 90.00° 96.55° 90.00°	Depositor
Resolution (Å)	48.92 – 2.30 48.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.92-2.30) 99.4 (48.92-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.216 , 0.241 0.217 , 0.241	Depositor DCC
R_{free} test set	1743 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4240	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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: ZN

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	0.35	0/2122	0.56	2/2896 (0.1%)
1	B	0.33	0/2149	0.54	0/2933
All	All	0.34	0/4271	0.55	2/5829 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	GLU	OE1-CD-OE2	6.76	131.41	123.30
1	A	292	ILE	CG1-CB-CG2	-6.64	96.79	111.40

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	2081	0	2003	49	0
1	B	2106	0	2023	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	22	0	0	0	0
3	B	29	0	0	0	0
All	All	4240	0	4026	86	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 10.

All (86) 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:292:ILE:HG22	1:A:296:ARG:NH1	1.60	1.15
1:A:292:ILE:HG22	1:A:296:ARG:CZ	1.97	0.94
1:A:292:ILE:C	1:A:296:ARG:NH2	2.30	0.85
1:A:292:ILE:CG2	1:A:296:ARG:NH1	2.39	0.85
1:A:293:ALA:HA	1:A:296:ARG:HH21	1.56	0.71
1:B:222:GLN:NE2	1:B:228:SER:O	2.26	0.68
1:A:250:ILE:HD12	1:A:265:ALA:HA	1.76	0.68
1:B:268:ALA:HB1	1:B:270:LEU:HD23	1.76	0.67
1:A:293:ALA:CA	1:A:296:ARG:HH21	2.08	0.67
1:A:293:ALA:N	1:A:296:ARG:NH2	2.43	0.66
1:A:293:ALA:N	1:A:296:ARG:HH21	1.94	0.65
1:A:292:ILE:CG2	1:A:296:ARG:HH12	2.08	0.65
1:A:147:LYS:NZ	1:A:180:ASP:OD1	2.30	0.64
1:B:201:VAL:CG1	1:B:250:ILE:HG13	2.28	0.64
1:A:149:TYR:O	1:A:153:ILE:HG12	1.99	0.62
1:B:143:VAL:HG12	1:B:214:TYR:OH	1.98	0.62
1:A:82:ASN:O	1:A:107:THR:OG1	2.14	0.62
1:A:187:ARG:NH2	1:A:213:ALA:O	2.33	0.61
1:B:190:ILE:HG21	1:B:214:TYR:O	1.99	0.61
1:B:185:GLU:OE1	1:B:296:ARG:NH1	2.33	0.61
1:A:114:GLU:HB3	1:A:130:PHE:HZ	1.65	0.61
1:A:84:LEU:HD11	1:A:107:THR:HG21	1.83	0.60
1:B:201:VAL:HG11	1:B:250:ILE:HG13	1.84	0.60
1:B:147:LYS:NZ	1:B:180:ASP:OD1	2.36	0.58
1:A:80:LEU:HD13	1:A:153:ILE:HD12	1.84	0.58
1:A:31:ALA:HB1	1:A:36:ILE:HG13	1.86	0.58
1:B:197:ARG:HH21	1:B:306:LEU:HA	1.69	0.58
1:A:122:HIS:O	1:A:123:TYR:HB3	2.07	0.54
1:A:250:ILE:HD12	1:A:265:ALA:CA	2.37	0.54
1:B:143:VAL:HG13	1:B:144:PRO:HD3	1.90	0.54
1:A:113:MET:HE1	1:A:209:TYR:HA	1.91	0.53
1:B:199:THR:HG22	1:B:217:HIS:HB2	1.91	0.52
1:B:201:VAL:HG12	1:B:250:ILE:HA	1.90	0.52
1:A:183:ASP:O	1:A:187:ARG:HG3	2.09	0.51
1:A:242:ILE:HG23	1:A:247:ALA:HB3	1.92	0.51
1:B:81:THR:O	1:B:106:LEU:HG	2.10	0.51
1:A:118:GLY:HA3	1:B:245:ARG:HH12	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:GLU:N	1:B:26:PRO:HD2	2.26	0.51
1:A:292:ILE:O	1:A:296:ARG:NH2	2.44	0.50
1:A:196:ASP:O	1:A:197:ARG:HD2	2.13	0.48
1:B:68:ALA:HA	1:B:71:ILE:HD12	1.96	0.48
1:A:292:ILE:C	1:A:296:ARG:HH21	2.11	0.47
1:B:194:PRO:O	1:B:198:ARG:HD3	2.12	0.47
1:B:31:ALA:HB1	1:B:36:ILE:HG13	1.95	0.47
1:B:193:LEU:O	1:B:198:ARG:NH1	2.47	0.47
1:B:288:ALA:HB1	1:B:294:MET:HB2	1.97	0.47
1:A:64:GLU:HA	1:A:65:PRO:HD3	1.68	0.47
1:A:201:VAL:CG1	1:A:250:ILE:HG12	2.46	0.46
1:A:204:HIS:CE1	1:A:255:ILE:HD11	2.49	0.46
1:B:113:MET:HE1	1:B:209:TYR:HA	1.97	0.46
1:B:158:CYS:HB3	1:B:165:CYS:HB2	1.35	0.46
1:B:116:PRO:HD3	1:B:208:ARG:CZ	2.46	0.46
1:A:190:ILE:HG21	1:A:214:TYR:O	2.16	0.46
1:B:66:ARG:HG2	1:B:69:ASP:OD2	2.16	0.46
1:B:197:ARG:HE	1:B:197:ARG:HB3	1.53	0.45
1:B:242:ILE:HG23	1:B:247:ALA:HB3	1.98	0.45
1:B:203:ALA:O	1:B:221:PRO:HD2	2.16	0.45
1:B:252:ALA:HA	1:B:261:LEU:HD13	1.99	0.45
1:A:292:ILE:HG22	1:A:296:ARG:NH2	2.32	0.44
1:B:250:ILE:HD13	1:B:270:LEU:HB2	1.99	0.44
1:A:199:THR:HB	1:A:247:ALA:HA	1.99	0.44
1:A:292:ILE:O	1:A:296:ARG:CZ	2.65	0.44
1:A:296:ARG:HB2	1:A:296:ARG:HE	1.33	0.44
1:B:143:VAL:HG23	1:B:179:LEU:HD22	1.99	0.44
1:A:201:VAL:HA	1:A:219:LEU:O	2.18	0.44
1:A:120:HIS:CD2	1:A:121:TYR:HB2	2.54	0.43
1:A:132:ALA:HA	1:A:133:GLY:HA2	1.69	0.43
1:A:196:ASP:C	1:A:197:ARG:HD2	2.39	0.42
1:A:288:ALA:HB1	1:A:294:MET:HB2	2.01	0.42
1:A:114:GLU:HB3	1:A:130:PHE:CZ	2.50	0.42
1:A:292:ILE:HD13	1:A:292:ILE:HG21	1.57	0.42
1:B:204:HIS:CE1	1:B:206:ALA:HB2	2.54	0.42
1:A:81:THR:HG21	1:A:90:LEU:HD21	2.02	0.42
1:B:131[B]:HIS:O	1:B:132:ALA:HB3	2.19	0.42
1:A:118:GLY:HA3	1:B:245:ARG:NH1	2.34	0.42
1:B:137:PRO:O	1:B:139:ALA:N	2.44	0.42
1:B:145:ASN:O	1:B:149:TYR:HD1	2.03	0.41
1:A:113:MET:HE3	1:A:209:TYR:CG	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:SER:OG	1:A:227:GLU:HG3	2.20	0.41
1:B:245:ARG:HB3	1:B:245:ARG:HE	1.76	0.41
1:A:117:GLY:HA2	1:A:118:GLY:HA2	1.60	0.41
1:A:252:ALA:HA	1:A:261:LEU:HD13	2.03	0.41
1:B:147:LYS:HA	1:B:150:VAL:HG22	2.02	0.41
1:B:197:ARG:NH2	1:B:248:SER:HB3	2.35	0.41
1:A:144:PRO:HB2	1:B:128:ALA:HB2	2.03	0.41
1:B:39:PHE:HB3	1:B:153:ILE:HD12	2.03	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	282/286 (99%)	265 (94%)	12 (4%)	5 (2%)	8	7
1	B	284/286 (99%)	265 (93%)	13 (5%)	6 (2%)	7	5
All	All	566/572 (99%)	530 (94%)	25 (4%)	11 (2%)	7	7

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	TYR
1	A	117	GLY
1	A	131	HIS
1	A	135	HIS
1	B	133	GLY
1	B	132	ALA
1	B	134	ALA
1	B	98	GLY
1	B	128	ALA
1	A	123	TYR

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Mol	Chain	Res	Type
1	B	138	HIS

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	198/200 (99%)	195 (98%)	3 (2%)	65	79
1	B	201/200 (100%)	197 (98%)	4 (2%)	55	72
All	All	399/400 (100%)	392 (98%)	7 (2%)	59	75

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ARG
1	A	130	PHE
1	A	234	ASP
1	B	91	THR
1	B	121	TYR
1	B	158	CYS
1	B	243	ARG

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

Mol	Chain	Res	Type
1	A	169	GLN
1	B	222	GLN
1	B	263	GLN

5.3.3 RNA ⓘ

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	284/286 (99%)	0.79	30 (10%) 6 8	41, 65, 118, 158	0
1	B	284/286 (99%)	0.74	19 (6%) 17 23	47, 74, 111, 141	0
All	All	568/572 (99%)	0.77	49 (8%) 10 14	41, 70, 115, 158	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	LYS	10.1
1	B	124	ILE	6.0
1	A	119	GLY	5.8
1	A	121	TYR	5.4
1	A	232	ALA	5.4
1	A	233	ALA	4.8
1	A	118	GLY	4.7
1	A	131	HIS	4.4
1	A	134	ALA	3.8
1	B	123	TYR	3.7
1	B	125	ASP	3.5
1	B	98	GLY	3.4
1	A	123	TYR	3.3
1	B	197	ARG	3.1
1	A	271	PRO	3.1
1	A	234	ASP	3.1
1	A	125	ASP	3.0
1	B	126	GLY	3.0
1	B	307	ALA	2.9
1	A	120	HIS	2.8
1	A	127	LYS	2.8
1	B	128	ALA	2.7
1	A	128	ALA	2.7
1	A	132	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	267	GLU	2.6
1	B	271	PRO	2.6
1	A	236	ALA	2.5
1	A	296	ARG	2.4
1	A	191	ALA	2.4
1	A	230	ALA	2.3
1	B	102	ALA	2.3
1	A	71	ILE	2.3
1	B	270	LEU	2.3
1	A	231	ALA	2.3
1	A	235	VAL	2.2
1	B	191	ALA	2.2
1	B	75	GLY	2.2
1	A	268	ALA	2.1
1	A	129	VAL	2.1
1	B	74	ALA	2.1
1	B	190	ILE	2.1
1	A	259	ARG	2.1
1	A	74	ALA	2.1
1	B	266	ARG	2.1
1	A	130	PHE	2.1
1	A	240	ARG	2.0
1	A	192	ALA	2.0
1	B	306	LEU	2.0
1	A	248	SER	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
2	ZN	B	401	1/1	0.99	0.20	46,46,46,46	0
2	ZN	A	401	1/1	0.99	0.19	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.