



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 05:24 PM UTC

PDB ID : 8EGK / pdb_00008egk
Title : Re-refinement of Crystal Structure of NosGet3d, the All4481 protein from Nostoc sp. PCC 7120
Authors : Barlow, A.N.; Manu, M.S.; Ramasamy, S.; Clemons Jr., W.M.
Deposited on : 2022-09-12
Resolution : 1.98 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

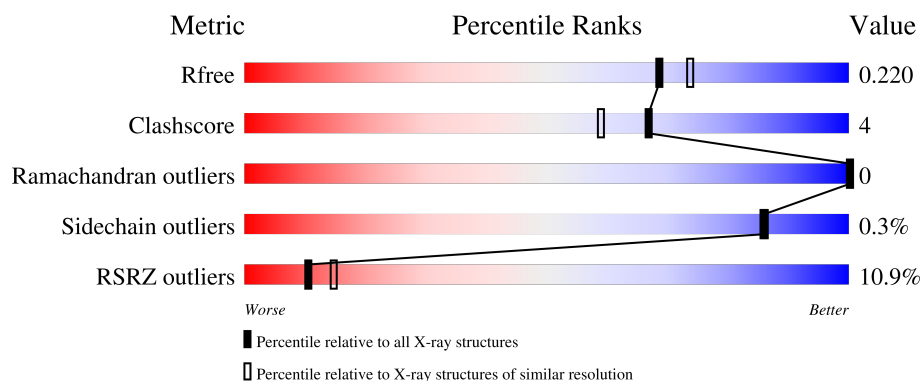
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	374	
1	B	374	

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	AZI	A	1101	-	X	-	-
2	AZI	B	1101	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11536 atoms, of which 5663 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 All4481 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	355	Total	C	H	N	O	Se	0	1	0
			5599	1784	2833	464	516	2			
1	B	355	Total	C	H	N	O	Se	0	0	0
			5592	1781	2830	463	516	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	THR	ALA	engineered mutation	UNP Q8YNT0
A	367	LEU	-	expression tag	UNP Q8YNT0
A	368	GLU	-	expression tag	UNP Q8YNT0
A	369	HIS	-	expression tag	UNP Q8YNT0
A	370	HIS	-	expression tag	UNP Q8YNT0
A	371	HIS	-	expression tag	UNP Q8YNT0
A	372	HIS	-	expression tag	UNP Q8YNT0
A	373	HIS	-	expression tag	UNP Q8YNT0
A	374	HIS	-	expression tag	UNP Q8YNT0
B	127	THR	ALA	engineered mutation	UNP Q8YNT0
B	367	LEU	-	expression tag	UNP Q8YNT0
B	368	GLU	-	expression tag	UNP Q8YNT0
B	369	HIS	-	expression tag	UNP Q8YNT0
B	370	HIS	-	expression tag	UNP Q8YNT0
B	371	HIS	-	expression tag	UNP Q8YNT0
B	372	HIS	-	expression tag	UNP Q8YNT0
B	373	HIS	-	expression tag	UNP Q8YNT0
B	374	HIS	-	expression tag	UNP Q8YNT0

- Molecule 2 is AZIDE ION (CCD ID: AZI) (formula: N₃).



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

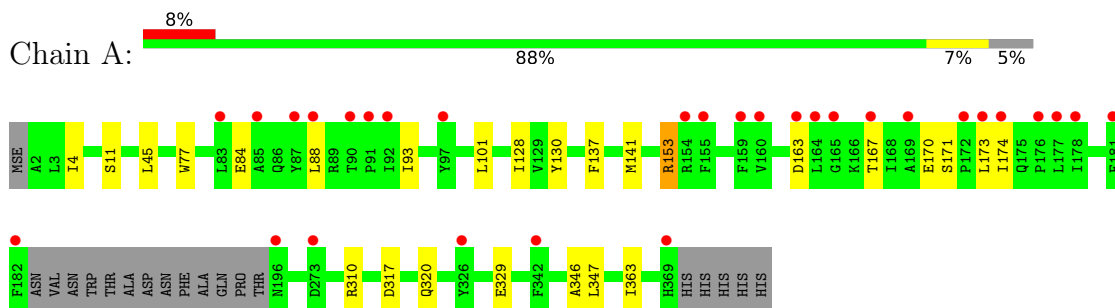
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	199	Total O 199 199	0	0
3	B	140	Total O 140 140	0	0

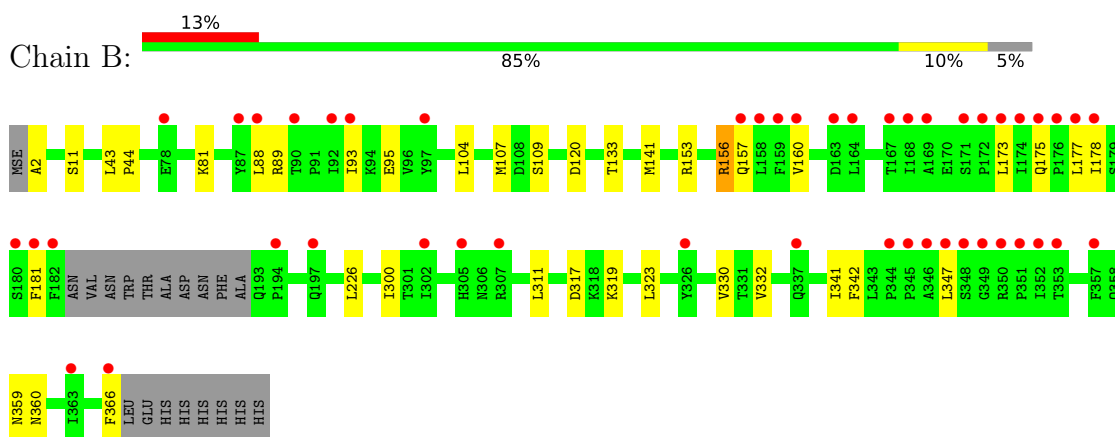
3 Residue-property plots [i](#)

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: All4481 protein



- Molecule 1: All4481 protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.17Å 55.55Å 122.36Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	27.52 – 1.98 27.52 – 1.98	Depositor EDS
% Data completeness (in resolution range)	94.3 (27.52-1.98) 94.3 (27.52-1.98)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, REFMAC Unknown, CNS	Depositor
R, R_{free}	0.189 , 0.221 0.189 , 0.220	Depositor DCC
R_{free} test set	2745 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11536	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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: AZI

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	0/2826	0.45	0/3844
1	B	0.30	0/2816	0.40	0/3832
All	All	0.32	0/5642	0.42	0/7676

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	ARG	Sidechain
1	B	153	ARG	Sidechain
1	B	156	ARG	Sidechain

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	2766	2833	2827	18	0
1	B	2762	2830	2830	27	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	199	0	0	0	0
3	B	140	0	0	0	0
All	All	5873	5663	5657	41	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 4.

All (41) 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:163:ASP:O	1:A:167:THR:HG23	1.96	0.66
1:B:323:LEU:HD12	1:B:332:VAL:HG22	1.87	0.56
1:B:330:VAL:HG13	1:B:341:ILE:HD12	1.89	0.55
1:B:330:VAL:CG1	1:B:341:ILE:HD12	2.36	0.55
1:A:153:ARG:HG2	1:A:153:ARG:HH11	1.72	0.53
1:A:130:TYR:CE2	1:A:141:MSE:HE1	2.45	0.52
1:B:88:LEU:HD12	1:B:89:ARG:N	2.25	0.52
1:A:137:PHE:CE2	1:B:133:THR:HG21	2.46	0.51
1:A:84:GLU:CG	1:A:88:LEU:HD12	2.42	0.50
1:B:323:LEU:CD1	1:B:332:VAL:HG22	2.41	0.49
1:A:174:ILE:HG22	1:B:177:LEU:HD11	1.96	0.48
1:B:88:LEU:HD12	1:B:89:ARG:H	1.78	0.47
1:A:153:ARG:NH2	1:A:329:GLU:OE2	2.48	0.47
1:B:109:SER:HB3	1:B:141:MSE:HG3	1.97	0.47
1:B:175:GLN:OE1	1:B:178:ILE:HD11	2.13	0.47
1:A:84:GLU:HG3	1:A:88:LEU:HD12	1.98	0.46
1:B:157:GLN:HA	1:B:157:GLN:OE1	2.16	0.46
1:B:317:ASP:OD1	1:B:317:ASP:C	2.58	0.45
1:B:156:ARG:O	1:B:160:VAL:HG13	2.17	0.45
1:B:342:PHE:C	1:B:342:PHE:CD1	2.95	0.45
1:A:45:LEU:HD23	1:B:226:LEU:HD23	1.99	0.45
1:B:95:GLU:HA	1:B:95:GLU:OE1	2.17	0.44
1:B:2:ALA:N	1:B:120:ASP:OD1	2.52	0.43
1:A:346:ALA:C	1:A:347:LEU:HD12	2.44	0.43
1:B:317:ASP:OD1	1:B:319:LYS:N	2.49	0.43
1:B:342:PHE:C	1:B:342:PHE:HD1	2.26	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:LEU:HD22	1:B:366:PHE:CG	2.53	0.43
1:A:310:ARG:NH1	1:A:363:ILE:HD11	2.34	0.43
1:B:89:ARG:HG2	1:B:181:PHE:HA	2.01	0.43
1:A:84:GLU:HG2	1:A:88:LEU:HD12	2.01	0.42
1:B:359:ASN:O	1:B:360:ASN:HB2	2.19	0.42
1:B:81:LYS:HG2	1:B:93:ILE:HD12	2.01	0.42
1:B:104:LEU:O	1:B:107:MSE:HB3	2.21	0.41
1:A:170:GLU:O	1:A:171:SER:C	2.63	0.41
1:B:43:LEU:HB3	1:B:44:PRO:HD3	2.02	0.41
1:A:4:ILE:HD13	1:A:128:ILE:HB	2.03	0.41
1:A:173:LEU:HD23	1:B:173:LEU:HD23	2.03	0.41
1:A:77:TRP:CD2	1:A:101:LEU:HD11	2.56	0.41
1:A:317:ASP:OD1	1:A:320:GLN:HG3	2.21	0.41
1:B:300:ILE:HD12	1:B:311:LEU:HD21	2.02	0.40
1:A:93:ILE:C	1:A:93:ILE:HD12	2.47	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	352/374 (94%)	344 (98%)	8 (2%)	0	100	100
1	B	351/374 (94%)	344 (98%)	7 (2%)	0	100	100
All	All	703/748 (94%)	688 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	303/316 (96%)	302 (100%)	1 (0%)	86	86
1	B	302/316 (96%)	301 (100%)	1 (0%)	86	86
All	All	605/632 (96%)	603 (100%)	2 (0%)	86	86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	B	11	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	B	29	GLN
1	B	49	GLN
1	B	76	ASN
1	B	196	ASN
1	B	280	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	AZI	B	1101	-	2,2,2	2.96	2 (100%)	0,1,1	-	-
2	AZI	A	1101	-	2,2,2	3.01	2 (100%)	0,1,1	-	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	AZI	N3-N2	-3.18	1.16	1.23
2	A	1101	AZI	N3-N2	-3.05	1.16	1.23
2	A	1101	AZI	N1-N2	-2.98	1.17	1.23
2	B	1101	AZI	N1-N2	-2.71	1.17	1.23

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

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	353/374 (94%)	0.10	30 (8%) 16 23	20, 33, 97, 119	0
1	B	353/374 (94%)	0.51	47 (13%) 7 10	26, 42, 103, 119	0
All	All	706/748 (94%)	0.31	77 (10%) 10 15	20, 38, 101, 119	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	366	PHE	5.8
1	B	182	PHE	4.8
1	A	164	LEU	4.6
1	A	87	TYR	4.5
1	B	172	PRO	4.3
1	B	347	LEU	4.3
1	B	176	PRO	4.1
1	A	169	ALA	4.1
1	A	174	ILE	4.0
1	B	326	TYR	4.0
1	B	181	PHE	3.9
1	A	173	LEU	3.8
1	B	88	LEU	3.8
1	B	351	PRO	3.8
1	A	181	PHE	3.7
1	A	97	TYR	3.7
1	B	160	VAL	3.7
1	A	182	PHE	3.7
1	A	167	THR	3.6
1	B	164	LEU	3.6
1	A	159	PHE	3.5
1	B	178	ILE	3.5
1	B	169	ALA	3.5
1	B	168	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	177	LEU	3.2
1	B	173	LEU	3.2
1	B	349	GLY	3.2
1	A	85	ALA	3.1
1	B	92	ILE	3.1
1	B	174	ILE	3.1
1	B	180	SER	3.1
1	B	159	PHE	3.0
1	B	352	ILE	3.0
1	B	348	SER	2.9
1	B	163	ASP	2.9
1	A	177	LEU	2.9
1	B	337	GLN	2.9
1	A	88	LEU	2.9
1	B	305	HIS	2.8
1	A	176	PRO	2.8
1	A	160	VAL	2.8
1	A	369	HIS	2.7
1	B	194	PRO	2.7
1	B	87	TYR	2.6
1	B	350	ARG	2.6
1	B	346	ALA	2.6
1	B	90	THR	2.6
1	B	157	GLN	2.6
1	A	172	PRO	2.6
1	B	353	THR	2.6
1	A	91	PRO	2.5
1	B	357	PHE	2.5
1	B	302	ILE	2.5
1	B	344	PRO	2.5
1	B	307	ARG	2.4
1	B	97	TYR	2.4
1	A	178	ILE	2.4
1	A	165	GLY	2.4
1	A	196	ASN	2.3
1	A	92	ILE	2.3
1	B	345	PRO	2.3
1	A	83	LEU	2.3
1	B	171	SER	2.2
1	A	90	THR	2.2
1	B	167	THR	2.2
1	A	155	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	342	PHE	2.2
1	A	273	ASP	2.2
1	B	93	ILE	2.1
1	A	154	ARG	2.1
1	B	197	GLN	2.1
1	A	163	ASP	2.1
1	B	363	ILE	2.1
1	B	78	GLU	2.1
1	B	158	LEU	2.1
1	B	175	GLN	2.0
1	A	326	TYR	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	AZI	B	1101	3/3	0.85	0.14	32,32,39,48	0
2	AZI	A	1101	3/3	0.90	0.14	37,37,39,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.