Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 06:54 PM EDT

PDB ID	:	2G29
Title	:	crystal structure of the periplasmic nitrate-binding protein NrtA from Synechocystis PCC 6803
Authors	:	Koropatkin, N.M.; Pakrasi, H.B.; Smith, T.J.
Deposited on	:	2006-02-15
Resolution	:	1.50 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 (i) 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 (i)) were used in the production of this report:

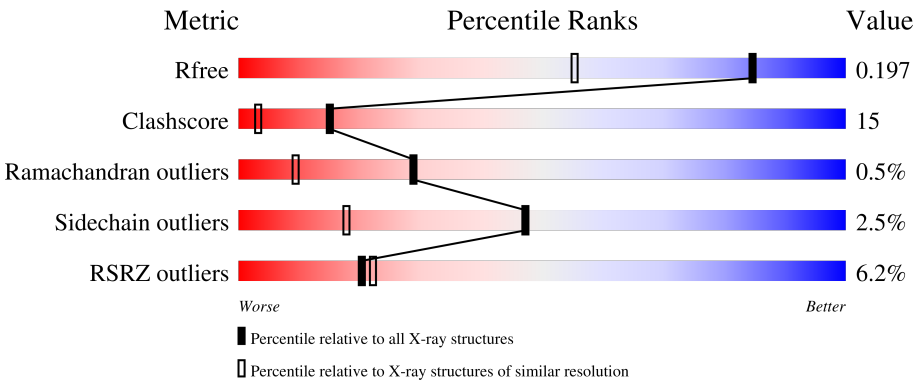
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

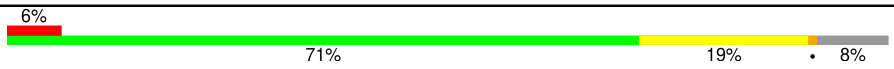
The reported resolution of this entry is 1.50 Å.

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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 <=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	417	

2 Entry composition (i)

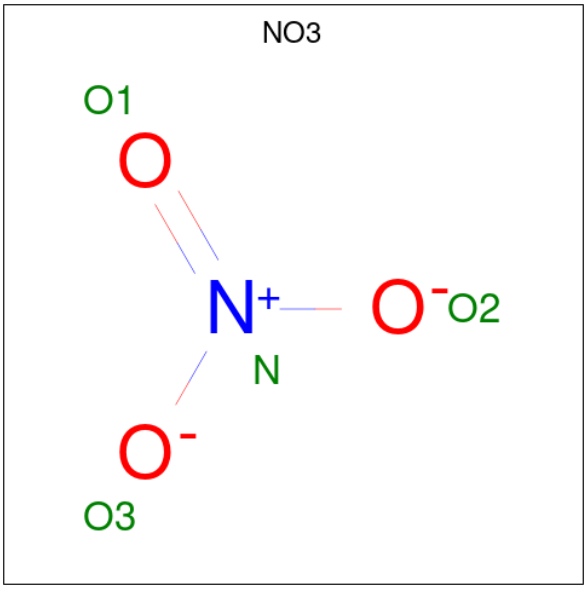
There are 3 unique types of molecules in this entry. The entry contains 3234 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nitrate transport protein nrtA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	3015	1929	498	571	17	0	0	0

- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
2	A	1	4	1	3	0	0

- Molecule 3 is water.

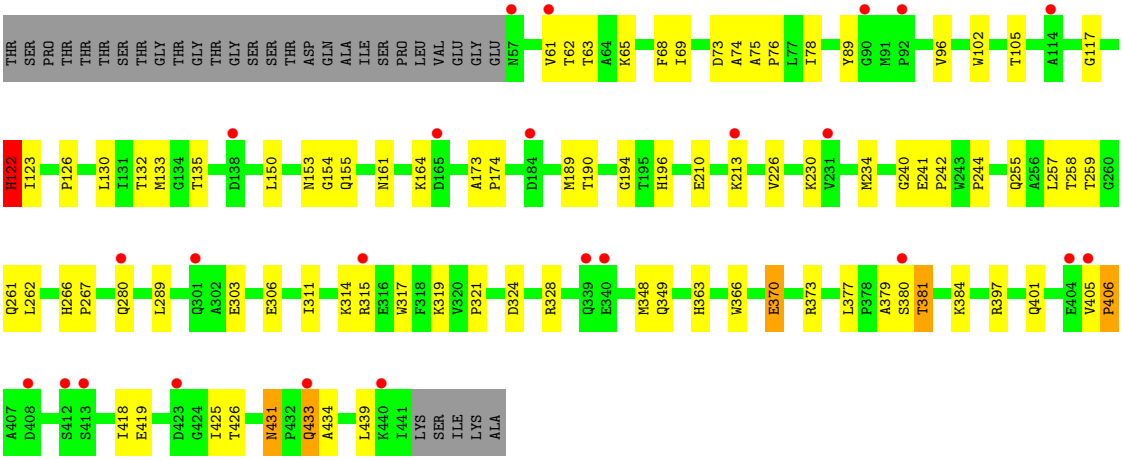
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	215	215	215	0	0

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: Nitrate transport protein nrtA

Chain A: 6% 71% 19% • 8%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.96Å 53.80Å 65.88Å 90.00° 107.67° 90.00°	Depositor
Resolution (Å)	50.00 – 1.50 23.89 – 1.51	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.50) 98.3 (23.89-1.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.91 (at 1.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.201 , 0.222 0.198 , 0.197	Depositor DCC
R_{free} test set	2947 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	12.1	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3234	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NO3

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	0.61	0/3095	0.76	1/4211 (0.0%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	122	HIS	N-CA-C	-6.24	94.17	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	TYR	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	3015	0	2938	90	0
2	A	4	0	0	0	0
3	A	215	0	0	13	0
All	All	3234	0	2938	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 15.

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:A:366:TRP:CZ2	1:A:370:GLU:HG2	1.89	1.06
1:A:431:ASN:HD21	1:A:433:GLN:HG2	1.26	0.95
1:A:155:GLN:HE21	1:A:196:HIS:HE1	1.00	0.91
1:A:155:GLN:HE21	1:A:196:HIS:CE1	1.92	0.80
1:A:431:ASN:ND2	1:A:433:GLN:HG2	1.96	0.79
1:A:405:VAL:O	1:A:406:PRO:O	2.01	0.78
1:A:61:VAL:HG12	1:A:63:THR:H	1.46	0.78
1:A:366:TRP:CH2	1:A:370:GLU:HG2	2.18	0.77
1:A:321:PRO:HG2	1:A:324:ASP:OD2	1.86	0.76
1:A:255:GLN:HE22	1:A:328:ARG:HH12	1.33	0.74
1:A:418:ILE:HG23	1:A:426:THR:HG23	1.73	0.71
1:A:155:GLN:NE2	1:A:196:HIS:HE1	1.84	0.70
1:A:126:PRO:HG2	1:A:194:GLY:HA2	1.73	0.70
1:A:315:ARG:HH11	1:A:319:LYS:HG2	1.57	0.69
1:A:76:PRO:HG2	1:A:150:LEU:HD22	1.76	0.68
1:A:405:VAL:O	1:A:405:VAL:HG12	1.94	0.67
1:A:280:GLN:HG3	3:A:878:HOH:O	1.95	0.66
1:A:226:VAL:O	1:A:230:LYS:HG3	1.96	0.65
1:A:258:THR:H	1:A:261:GLN:HE21	1.45	0.63
1:A:65:LYS:HE3	1:A:117:GLY:O	1.99	0.63
1:A:154:GLY:HA3	1:A:349:GLN:HG3	1.81	0.62
1:A:431:ASN:HD21	1:A:433:GLN:CG	2.06	0.62
1:A:366:TRP:CZ2	1:A:370:GLU:CG	2.75	0.62
1:A:348:MET:HE2	3:A:710:HOH:O	2.01	0.61
1:A:425:ILE:HD13	1:A:439:LEU:HD23	1.82	0.60
1:A:418:ILE:CG2	1:A:426:THR:HG23	2.31	0.60
1:A:380:SER:O	1:A:381:THR:C	2.40	0.60
1:A:418:ILE:HG23	1:A:426:THR:CG2	2.32	0.59
1:A:311:ILE:HA	1:A:314:LYS:HE3	1.84	0.59
1:A:73:ASP:OD1	1:A:122:HIS:HE1	1.85	0.59
1:A:363:HIS:HE1	1:A:419:GLU:OE2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:PRO:CG	1:A:150:LEU:HD22	2.34	0.58
1:A:363:HIS:HD2	3:A:706:HOH:O	1.87	0.57
1:A:154:GLY:HA3	1:A:349:GLN:CG	2.35	0.57
1:A:96:VAL:CG1	1:A:317:TRP:CH2	2.88	0.57
1:A:96:VAL:CG1	1:A:317:TRP:HH2	2.18	0.56
1:A:366:TRP:CH2	1:A:370:GLU:CG	2.87	0.56
1:A:96:VAL:HG11	1:A:317:TRP:CH2	2.41	0.55
1:A:96:VAL:O	1:A:96:VAL:HG13	2.05	0.55
1:A:303:GLU:H	1:A:303:GLU:CD	2.09	0.55
1:A:379:ALA:O	1:A:380:SER:HB2	2.07	0.54
1:A:259:THR:OG1	1:A:266:HIS:HE1	1.91	0.54
1:A:258:THR:H	1:A:261:GLN:NE2	2.06	0.53
1:A:384:LYS:HG2	3:A:865:HOH:O	2.09	0.53
1:A:373:ARG:HD3	3:A:842:HOH:O	2.08	0.52
1:A:69:ILE:H	1:A:122:HIS:HD2	1.57	0.52
1:A:418:ILE:CG2	1:A:426:THR:CG2	2.88	0.51
1:A:173:ALA:N	1:A:174:PRO:HD2	2.26	0.51
1:A:258:THR:HG22	1:A:261:GLN:HE21	1.76	0.50
1:A:69:ILE:HD12	1:A:69:ILE:N	2.27	0.50
1:A:68:PHE:C	1:A:69:ILE:HD12	2.32	0.50
1:A:241:GLU:HA	1:A:244:PRO:HD2	1.95	0.49
1:A:153:ASN:HA	1:A:266:HIS:CE1	2.48	0.49
1:A:257:LEU:HD13	1:A:262:LEU:HG	1.94	0.49
1:A:306:GLU:HB3	3:A:914:HOH:O	2.13	0.49
1:A:366:TRP:CE2	1:A:370:GLU:HG2	2.43	0.49
1:A:69:ILE:HD11	1:A:105:THR:OG1	2.13	0.48
1:A:130:LEU:HD22	1:A:135:THR:HG21	1.94	0.48
1:A:397:ARG:O	1:A:401:GLN:NE2	2.47	0.48
1:A:78:ILE:HD12	1:A:78:ILE:N	2.29	0.48
1:A:75:ALA:N	1:A:76:PRO:HD2	2.29	0.48
1:A:69:ILE:H	1:A:122:HIS:CD2	2.32	0.48
1:A:431:ASN:C	1:A:431:ASN:HD22	2.17	0.47
1:A:377:LEU:HD23	3:A:890:HOH:O	2.14	0.47
1:A:133:MET:HG3	3:A:906:HOH:O	2.13	0.47
1:A:96:VAL:HG11	1:A:317:TRP:HH2	1.78	0.46
1:A:380:SER:O	1:A:381:THR:O	2.34	0.46
1:A:405:VAL:N	1:A:406:PRO:CD	2.77	0.46
1:A:69:ILE:N	1:A:69:ILE:CD1	2.79	0.46
1:A:405:VAL:O	1:A:406:PRO:C	2.54	0.45
1:A:74:ALA:O	1:A:78:ILE:HD13	2.17	0.45
1:A:210:GLU:CD	1:A:213:LYS:HD2	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLU:CD	3:A:842:HOH:O	2.55	0.44
1:A:161:ASN:OD1	1:A:164:LYS:HE3	2.18	0.43
1:A:405:VAL:O	1:A:405:VAL:CG1	2.64	0.43
1:A:96:VAL:HG12	3:A:832:HOH:O	2.17	0.43
1:A:132:THR:HB	3:A:906:HOH:O	2.19	0.43
1:A:190:THR:OG1	1:A:196:HIS:HD2	2.00	0.43
1:A:259:THR:OG1	1:A:266:HIS:CE1	2.71	0.43
1:A:306:GLU:HG2	3:A:908:HOH:O	2.18	0.43
1:A:155:GLN:HA	1:A:240:GLY:HA2	2.01	0.42
1:A:78:ILE:N	1:A:78:ILE:CD1	2.83	0.42
1:A:61:VAL:HG12	1:A:62:THR:N	2.35	0.41
1:A:65:LYS:CE	1:A:117:GLY:O	2.68	0.41
1:A:431:ASN:ND2	1:A:434:ALA:H	2.19	0.41
1:A:373:ARG:HB3	3:A:842:HOH:O	2.21	0.41
1:A:96:VAL:HG13	1:A:317:TRP:CH2	2.56	0.41
1:A:425:ILE:HD13	1:A:439:LEU:CD2	2.50	0.41
1:A:102:TRP:CZ3	1:A:123:ILE:HA	2.56	0.40
1:A:266:HIS:HD2	1:A:267:PRO:O	2.04	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	383/417 (92%)	366 (96%)	15 (4%)	2 (0%)	29 9

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	PRO
1	A	381	THR

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	317/343 (92%)	309 (98%)	8 (2%)	47 18

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	A	189	MET
1	A	234	MET
1	A	242	PRO
1	A	289	LEU
1	A	370	GLU
1	A	431	ASN
1	A	433	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	A	155	GLN
1	A	158	GLN
1	A	196	HIS
1	A	250	GLN
1	A	255	GLN
1	A	261	GLN
1	A	266	HIS
1	A	301	GLN
1	A	355	ASN
1	A	363	HIS
1	A	401	GLN
1	A	431	ASN
1	A	433	GLN

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)

1 ligand is 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	NO3	A	700	-	1,3,3	2.58	1 (100%)	0,3,3	-	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	NO3	O1-N	2.58	1.37	1.24

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 (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	385/417 (92%)	0.44	24 (6%) 20 22	9, 14, 26, 36	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	405	VAL	13.8
1	A	380	SER	8.7
1	A	404	GLU	5.5
1	A	57	ASN	4.1
1	A	340	GLU	3.7
1	A	423	ASP	3.4
1	A	165	ASP	3.4
1	A	61	VAL	3.0
1	A	408	ASP	2.9
1	A	412	SER	2.8
1	A	184	ASP	2.7
1	A	433	GLN	2.7
1	A	413	SER	2.6
1	A	138	ASP	2.6
1	A	280	GLN	2.5
1	A	339	GLN	2.5
1	A	231	VAL	2.4
1	A	301	GLN	2.4
1	A	92	PRO	2.4
1	A	90	GLY	2.3
1	A	213	LYS	2.3
1	A	315	ARG	2.3
1	A	440	LYS	2.2
1	A	114	ALA	2.2

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	NO3	A	700	4/4	0.97	0.09	11,12,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.