



Full wwPDB X-ray Structure Validation Report ⓘ

May 2, 2023 – 01:17 pm BST

PDB ID : 7BN2
Title : Clathrin heavy chain N-terminal domain bound to Non structured protein 3 from Eastern Equine Encephalitis Virus
Authors : Badgujar, D.C.; Dobritsch, D.
Deposited on : 2021-01-21
Resolution : 1.97 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.32.2
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) : 2.32.2

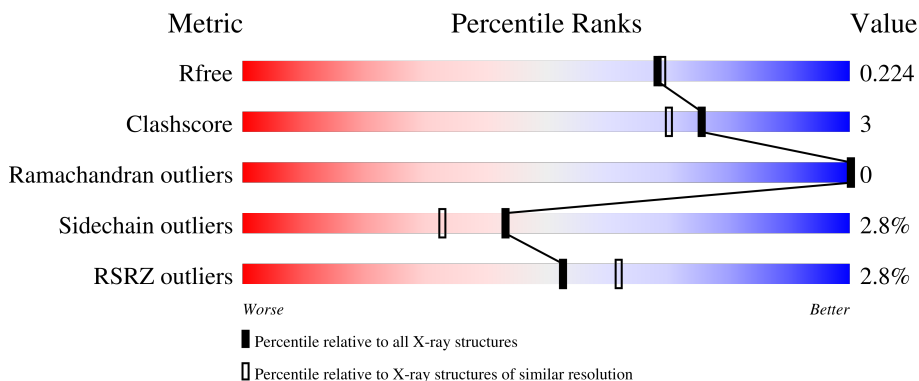
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

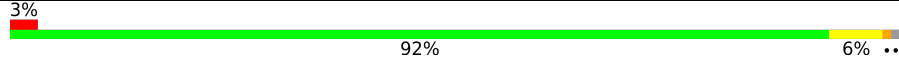
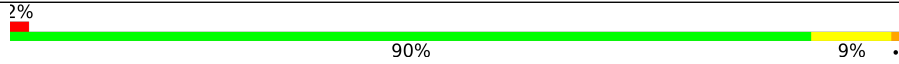
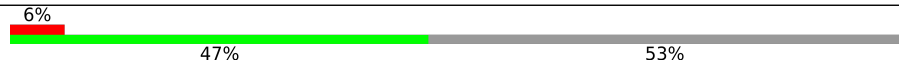
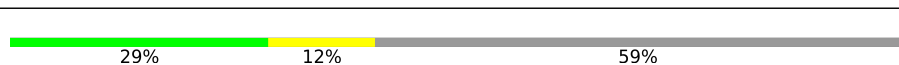
The reported resolution of this entry is 1.97 Å.

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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	AAA	364	 3% 92% 6% ..
1	BBB	364	 2% 90% 9% ..
2	CCC	17	 6% 47% 53%
2	DDD	17	 29% 12% 59%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6323 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 Clathrin heavy chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	361	2845	1812	487	526	20	0	5	0
1	BBB	361	2842	1807	488	528	19	0	4	0

- Molecule 2 is a protein called Non structured protein 3 from Eastern Equine Encephalitis Virus.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	CCC	8	63	41	8	14	0	0	0
2	DDD	7	57	38	7	12	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	BBB	1	Total	O	P	0	0
			5	4	1		

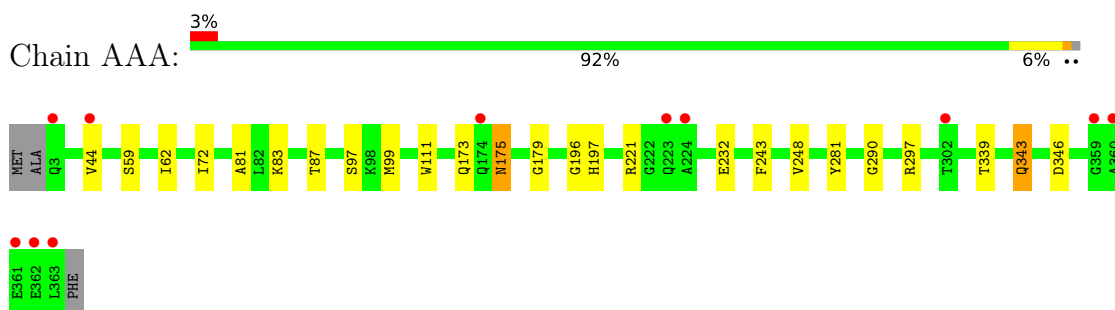
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	247	Total	O	0	2
			249	249		
5	BBB	246	Total	O	0	1
			247	247		
5	CCC	7	Total	O	0	0
			7	7		
5	DDD	3	Total	O	0	0
			3	3		

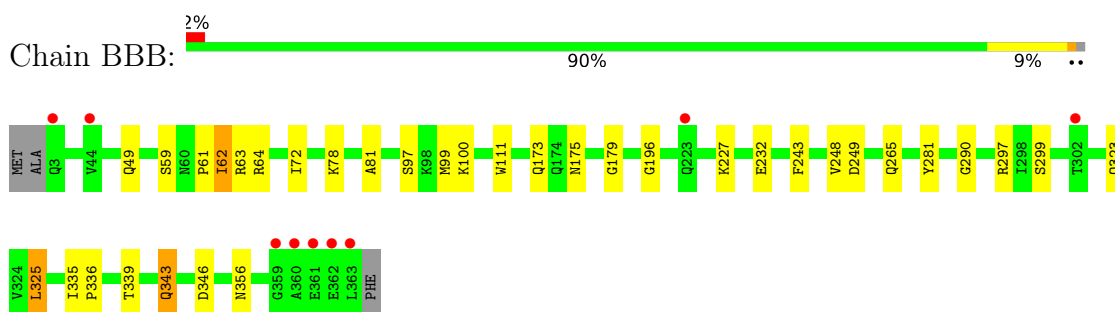
3 Residue-property plots [i](#)

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.

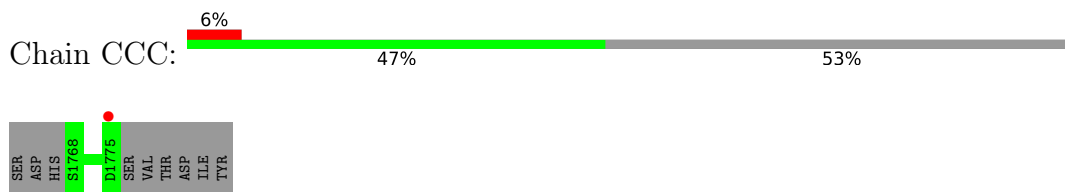
- Molecule 1: Clathrin heavy chain 1



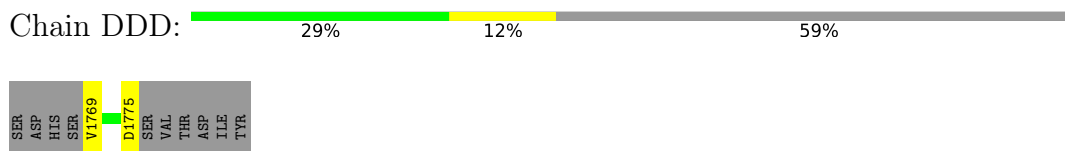
- Molecule 1: Clathrin heavy chain 1



- Molecule 2: Non structured protein 3 from Eastern Equine Encephalitis Virus



- Molecule 2: Non structured protein 3 from Eastern Equine Encephalitis Virus



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.90Å 129.12Å 77.88Å 90.00° 115.29° 90.00°	Depositor
Resolution (Å)	89.35 – 1.97 70.41 – 1.97	Depositor EDS
% Data completeness (in resolution range)	71.7 (89.35-1.97) 72.1 (70.41-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.97Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.181 , 0.219 0.188 , 0.224	Depositor DCC
R_{free} test set	3160 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtrriage
Anisotropy	0.111	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6323	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: PO4, SO4

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	AAA	0.68	0/2919	0.83	0/3957
1	BBB	0.68	0/2912	0.84	0/3948
2	CCC	0.69	0/63	0.83	0/85
2	DDD	0.74	0/57	0.86	0/77
All	All	0.68	0/5951	0.84	0/8067

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	2845	0	2867	12	0
1	BBB	2842	0	2859	25	0
2	CCC	63	0	59	0	0
2	DDD	57	0	54	0	0
3	AAA	5	0	0	0	0
4	BBB	5	0	0	0	0
5	AAA	249	0	0	0	0
5	BBB	247	0	0	3	0
5	CCC	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	DDD	3	0	0	0	0
All	All	6323	0	5839	36	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 3.

All (36) 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:BBB:62:ILE:HD11	1:BBB:64[A]:ARG:CZ	2.19	0.73
1:BBB:299:SER:HB3	5:BBB:647:HOH:O	1.87	0.72
1:BBB:323:GLN:OE1	1:BBB:325:LEU:HD22	1.98	0.64
1:AAA:97:SER:OG	1:AAA:99[B]:MET:CE	2.47	0.62
1:BBB:64[A]:ARG:HH21	1:BBB:64[A]:ARG:HG3	1.65	0.62
1:BBB:62:ILE:HG23	5:BBB:684:HOH:O	2.02	0.59
1:AAA:97:SER:OG	1:AAA:99[B]:MET:HE1	2.02	0.58
1:BBB:49:GLN:OE1	1:BBB:63:ARG:HD3	2.08	0.53
1:BBB:227:LYS:NZ	1:BBB:249:ASP:OD1	2.39	0.52
1:BBB:97:SER:OG	1:BBB:99[B]:MET:HE1	2.10	0.51
1:BBB:97:SER:OG	1:BBB:99[B]:MET:CE	2.58	0.51
1:BBB:72:ILE:HG13	1:BBB:81:ALA:HB3	1.93	0.50
1:BBB:232:GLU:HB2	1:BBB:243:PHE:HB3	1.93	0.49
1:BBB:62:ILE:HD11	1:BBB:64[B]:ARG:HG2	1.95	0.49
1:BBB:62:ILE:HD11	1:BBB:64[A]:ARG:NH2	2.28	0.49
1:BBB:62:ILE:HD11	1:BBB:64[A]:ARG:HG2	1.94	0.48
1:AAA:197[B]:HIS:HD2	1:AAA:221:ARG:H	1.61	0.48
1:AAA:339:THR:O	1:AAA:343:GLN:HA	2.13	0.48
1:AAA:175:ASN:OD1	1:BBB:356:ASN:HA	2.14	0.48
1:BBB:339:THR:O	1:BBB:343:GLN:HA	2.15	0.47
1:AAA:72:ILE:HG13	1:AAA:81:ALA:HB3	1.96	0.46
1:BBB:248:VAL:HG21	1:BBB:290:GLY:O	2.15	0.46
1:BBB:62:ILE:CD1	1:BBB:64[A]:ARG:CZ	2.91	0.46
1:BBB:265:GLN:HB3	5:BBB:654:HOH:O	2.16	0.46
1:BBB:179:GLY:HA3	1:BBB:196:GLY:O	2.15	0.46
1:AAA:44:VAL:HG23	1:AAA:44:VAL:O	2.16	0.45
1:BBB:62:ILE:HD11	1:BBB:64[A]:ARG:CG	2.48	0.43
1:BBB:59:SER:O	1:BBB:61:PRO:HD2	2.18	0.43
1:AAA:281:TYR:CZ	1:AAA:297:ARG:HD2	2.53	0.43
1:BBB:281:TYR:CZ	1:BBB:297:ARG:HD2	2.54	0.43
1:AAA:179:GLY:HA3	1:AAA:196:GLY:O	2.19	0.43
1:BBB:62:ILE:CG1	1:BBB:64[A]:ARG:NH2	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:83:LYS:HA	1:AAA:87:THR:O	2.20	0.42
1:BBB:335:ILE:HB	1:BBB:336:PRO:HD3	2.01	0.41
1:AAA:232:GLU:HB2	1:AAA:243:PHE:HB3	2.02	0.41
1:AAA:248:VAL:HG21	1:AAA:290:GLY:O	2.21	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	AAA	364/364 (100%)	359 (99%)	5 (1%)	0	100	100
1	BBB	363/364 (100%)	358 (99%)	5 (1%)	0	100	100
2	CCC	6/17 (35%)	6 (100%)	0	0	100	100
2	DDD	5/17 (29%)	5 (100%)	0	0	100	100
All	All	738/762 (97%)	728 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	314/311 (101%)	307 (98%)	7 (2%)	52	44
1	BBB	313/311 (101%)	304 (97%)	9 (3%)	42	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	CCC	8/17 (47%)	8 (100%)	0	100	100
2	DDD	7/17 (41%)	5 (71%)	2 (29%)	0	0
All	All	642/656 (98%)	624 (97%)	18 (3%)	43	33

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	59	SER
1	AAA	62	ILE
1	AAA	111	TRP
1	AAA	173	GLN
1	AAA	175	ASN
1	AAA	343	GLN
1	AAA	346	ASP
1	BBB	62	ILE
1	BBB	78	LYS
1	BBB	100	LYS
1	BBB	111	TRP
1	BBB	173	GLN
1	BBB	175	ASN
1	BBB	325	LEU
1	BBB	343	GLN
1	BBB	346	ASP
2	DDD	1769	VAL
2	DDD	1775	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

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
3	SO4	AAA	401	-	4,4,4	0.32	0	6,6,6	0.09	0
4	PO4	BBB	401	-	4,4,4	1.46	1 (25%)	6,6,6	0.57	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	401	PO4	P-O1	2.89	1.57	1.50

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	AAA	361/364 (99%)	-0.09	11 (3%) 50 59	20, 33, 59, 99	0
1	BBB	361/364 (99%)	-0.10	9 (2%) 57 66	18, 33, 57, 106	0
2	CCC	8/17 (47%)	0.10	1 (12%) 3 6	27, 34, 63, 90	0
2	DDD	7/17 (41%)	-0.23	0 100 100	28, 36, 47, 76	0
All	All	737/762 (96%)	-0.10	21 (2%) 53 62	18, 33, 61, 106	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	3	GLN	5.1
1	BBB	363	LEU	5.0
1	AAA	224	ALA	4.9
1	BBB	362	GLU	4.7
1	BBB	361	GLU	4.4
1	AAA	363	LEU	4.2
1	AAA	361	GLU	3.7
1	BBB	359	GLY	3.7
2	CCC	1775	ASP	3.6
1	AAA	302	THR	3.5
1	AAA	223	GLN	3.4
1	AAA	359	GLY	3.3
1	AAA	3	GLN	3.3
1	BBB	44	VAL	3.0
1	AAA	360	ALA	2.8
1	AAA	174	GLN	2.8
1	AAA	362	GLU	2.7
1	BBB	223	GLN	2.7
1	BBB	360	ALA	2.5
1	BBB	302	THR	2.3
1	AAA	44	VAL	2.3

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
3	SO4	AAA	401	5/5	0.88	0.18	84,91,104,107	0
4	PO4	BBB	401	5/5	0.98	0.08	40,45,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.